Institut für Theoretische Physik
Direktor: Prof. Dr. Frank Steiner

ulm university universität ulm

Semiclassics, adiabatic decoupling and perturbed periodic structures

Dissertation

zur Erlangung des Doktorgrades Dr. rer. nat.
der Fakultät für Naturwissenschaften
der Universität Ulm

vorgelegt von

Eric Sträng

aus Lund.

2008

Amtierenden Dekan: Prof. Dr. Peter Bäuerle
Erstgutachter: Prof. Dr. Jens Bolte
Zweitgutachter: Prof. Dr. Frank Steiner

Tag der Promotion: 9. Februar 2009

Preface

This thesis is an attempt to report the research I have conducted during the three years I have been active at the Institute of Theoretical Physics of the university in Ulm.

It has really been a privilege to work at the institute of theoretical physics. I would therefore like to thank all members and former members of the institute I have had the pleasure of meeting. In particular, I would like to thank Jens Bolte for his support and supervision the last three years and Frank Steiner for the friendly atmosphere he has created at the institute. I would also like to thank Stefan Keppeler for recommending me to the latter two.

I have had the pleasure to engage in many an interesting discussion at the department. I would like to commend Sebastian Endres, Konstantin Glaum, Holger Janzer, Maximilian Köpke, Raphael Lamon, Sven Lustig, Benjamin Obert, Wolfgang Peter, Stefan Poppe, Nils Bezares–Roder, Hans–Michael Stiepan, Alvise Verso, Daniel Waltner for their active participation. I am particular thankful to Raphael who has introduced me to quantum loop gravity.

I am also indebted to all the persons who have contributed to the proof reading of this thesis. Those include Nils Bezares-Roder, Sven Lustig, Sebastian Endres, Frank Steiner, Raphael Lamon and Jens Bolte. The largest part of the burden has been carried by Jens.

I would like to thank the graduate school "Analysis of complexity, information and evolution" of the Land Baden-Württemberg for the stipend which has permitted me to do this doctoral thesis. I would furthermore like to thank the members and professors of the graduate school. Amongst them I would particularly like to thank Wolfgang Arendt and Werner Balser of the Institute of Applied Analysis who have always been more than willing to assist me.

Last but not least, I would like to thank Anna, Axel and my parents whose contributions to this thesis, though not of scientific nature, have been highly appreciated.

Abstract

This thesis deals with the consequences of periodic structures in quantum mechanics. This is done first in the usual semiclassical, i.e., relating properties of classical mechanics and quantum mechanics. In a second step we study periodic Schrödinger operators.

The first chapter introduces the main tool for dealing with differential equations with periodic coefficients, namely, Floquet theory. As an example it is applied on the Hill equation. Hill equations appear in a class of spectral problem for certain Schrödinger operators with periodic potentials. As a special case, the solutions to the Mathieu equation are then studied exemplifying the properties of the corresponding spectrum. Special attention is brought to the properties of the spectrum and the corresponding Floquet exponent of the corresponding solution. This relation is given by the Whittaker formula which is explicit up to a term which can be characterized as the determinant of an infinite dimensional matrix. We present new results concerning this determinant. It is expressed as the limiting case of a third order recurrence to which we can write any term explicitly. To do this we present a novel procedure to represent any linear recurrence without constant terms.

After a short review of classical mechanics, we introduce quantum mechanics in the context of the Weyl quantization. In effect this gives us a bridge between classical dynamics and quantum mechanics. In particular, we introduce semiclassical propagation results which, up to some known errors, describes the propagation of an initial Gaußian under quantum evolution [CR97]. This approximation breaks down at what is commonly known as the Ehrenfest time. We use these results to investigate the localization properties of an initial Gaußian up to the Ehrenfest time. We can show localization of the state up to the Ehrenfest time under the assumption that the flow differential of the corresponding classical motion admits Floquet solutions with purely imaginary Floquet exponents. In this case, we also show the existence of what we call classical revivals which occur at multiples of the classical period. In the case of periodic classical motion, the classical period is nothing else but the period of the motion.

The last part is a study of the spectral properties of perturbed periodic Schrödinger operators. This is also done in the context of semiclassics, however, the perturbation parameter is now the strength of the perturbation ε. To do this we must consider operator valued Weyl calculus. We do this in the context of $\tau-$equivariant symbols [PST03]. As the structure of the band spectrum of the unperturbed operator remains unchanged under small enough perturbations, the effective dynamics can be described adiabatically under certain prerequisites. We consider the construction of multi-valued WKB ansätze [LF91, EW96]. Our results include Bohr-Sommerfeld quantization conditions modulo $\mathcal{O}\left(\varepsilon^2\right)$. Those are used to investigate the Wannier–Stark system. Such systems have been investigated numerically showing that its evolution is almost dispersionless when restricted to one band [HKKM04, WKKM04]. We show that this is due to the fact that the corresponding Berry phase of the WKB ansatz does not depend on the energy, such that, the spectrum of a particle restricted to one band is that of a harmonic oscillator modulo $\mathcal{O}\left(\varepsilon^2\right)$.

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Chapter 1

Introduction

This thesis is dedicated to the study of periodic, or close to periodic structures in mechanics. We consider the interplay of periodic structures in classical mechanics and their implications on quantum mechanics. More stringently, we consider the parallel between the properties of quantum systems and their classical analogs. The bridge between classical and quantum is implemented by the Weyl quantization, a semiclassical approach to quantum mechanics. The main aim is the study of quantum dynamics and the spectral properties of quantum operators.

In quantum mechanics, the time evolution is given by a unitary group that is characterized by the (real) eigenvalues of the Hamilton operator. In essence, one knows all about the evolution of any initial state if one has solved the corresponding spectral problem. This usually involves recognition and use of the symmetries of the quantum system. While computing eigenvalues is numerically feasible, one often has to resort to more specific approximations because of numerical errors. Furthermore, it is seldom possible to formulate qualitative statements about the evolved state, in particular, after long times.

Classical mechanics uses the concept of point particles. In contrast to quantum mechanics, this particle is coherent and localized for all times. Solutions of the classical evolutions are obtained by integration of Hamilton's equations of motion. Concepts of regularity and integrability are known permitting a characterization of the solutions. Integrable motion is at least quasi–periodic.

The quantum harmonic oscillator has a very special evolution in that the particles are propagated in a dispersionless manner. For generic quantum systems, it is known that the evolved state disperses which raises a legitimate question about the dispersion of evolved states. One question we ask ourselves is: do quantum states remain localized? The largest part of existing investigations has been developed in the opposite direction. One important result is the quantum ergodicity theorem [Šni74, CdV85, Zel87]. It states that almost all eigenfunc-

tions (the stable structures of quantum mechanics) of the Hamilton operator tend to equidistribute on phase space in the classical limit if the classical analog of the system is ergodic. Furthermore, it has been conjectured that evolved quantum states equidistribute on phase space if the corresponding classical system is chaotic [BB79, Sch05]. We recall that the classical limit is formally equivalent to studying the singular limit $\hbar \to 0$, where $\hbar$ denotes the Planck constant.

Now, Bohr's correspondence principle relates classical mechanics and quantum mechanics in the classical limit. How does one retrieve the classical and localized particle from an apparently ephemeral quantum particle? The question has been studied thoroughly using semiclassical methods [CR97, BR02, HJ99, HJ00]. The result can be put in the following form. In the classical limit, $\hbar \to 0$, a particle will be described by classical mechanics indefinitely. We rephrase at this point to emphasize the typical semiclassical statement. The times $T_E(\hbar)$ for which the particle is described by classical mechanics tends to infinity as $\hbar \to 0$. One of the question we will study in this thesis is just the localization properties of a quantum particle. Localization plays an important role in existing approximation which rely on the relation between classical and quantum mechanics.

One of the motivations to study localization has been numerical studies of certain systems. These apparently show that the evolution of localized particles remain localized and furthermore are periodic up to some small errors [HKKM04, WKKM04, GKK02]. The studied system was the so–called Wannier–Stark system. It is described by a periodic Schrödinger operator[1] with a linear perturbation in position. The unperturbed Schrödinger operator can be seen as a fibered Hamiltonian over the Brillouin zone where each fiber has discrete spectrum. Then, considering n^{th} eigenvalues of the fibers, one can describe an energy band over the Brillouin zone. The evolution of an initial Gaußian projected on such a band remains "almost dispersion-less" [HKKM04, WKKM04]. We attack this by considering the spectral properties of such Hamiltonians. In particular we seek WKB quasi–modes and corresponding resonances to the full Hamiltonian.

It should be noted that the Wannier–Stark systems have been realized experimentally. Such experiments, though not without controversy, have resolved the issue of Bloch oscillations [RS97] and the existence of the Wannier–Stark ladder of resonances [Wan60, Wan62, WF62]. So far, these have been realized with solid state devices, optical lattices and Bose-Einstein condensates.

Along this thesis, several concepts of periodicity will be used. The central concept is the usual one. Here $\mathbb{X}$ will be some Banach space with norm $||\cdot||$.

[1] The periodic potential is merely a cosine.

Definition 1.1 (Periodicity)**.** A function $f : \mathbb{R} \to \mathbb{X}$ satisfying

$$f(t+\tau) = f(t), \quad \forall t \in \mathbb{R}, \tag{1.1}$$

is called $\tau-$periodic.

A somewhat larger group of functions is that of quasi–periodic functions. They can be characterized in the following manner.

Definition 1.2 (Quasi–periodicity)**.** A function $f : \mathbb{R} \to \mathbb{X}$ that can be written as

$$f(t) = \sum_{j=1}^{N} c_j e^{i\omega_j t}, \quad N \in \mathbb{N}, \omega_j \in \mathbb{R}, c_j \in \mathbb{X}, \tag{1.2}$$

is called quasi–periodic.

Second periodic functions or Bloch functions are a special case of quasi–periodic functions which satisfy

$$f(t+\tau) = \varepsilon f(t), \quad \forall t \in R, \exists \varepsilon \in \mathbb{C}, \tau \in \mathbb{R}. \tag{1.3}$$

Periodic functions are also called first periodic in contrast to second periodic functions. The weakest concept of periodicity is almost periodicity.

Definition 1.3 (Almost-periodicity)**.** A function $f : \mathbb{R} \to \mathbb{X}$ satisfying

$$\forall \varepsilon > 0, \exists \tau \in \mathbb{R} \quad \text{such that} \quad ||f(t+\tau) - f(t)|| < \varepsilon, \tag{1.4}$$

is called almost periodic.

These functions were characterized by Harald Bohr [Boh24, Boh25].

This thesis is arranged as follows. Three main chapters introduce some of the obtained results. The first chapter is an introduction to the theory of Hill equations, i.e., the study of ordinary differential equation with periodic coefficients. This is done by introduction of the Floquet theorem which allows to study the spectrum of such differential equations. This chapter also serves as a general introduction to the thesis stating notation. Sections 2.4.4, 2.4.5, 2.4.6 are new while sections 2.4.2 and 2.4.3 are in some form revised versions of existing descriptions.

The second chapter is intended as a short summary on classical methods. As many of the methods later used refer to classical mechanics, such a review seems appropriate. The intent is to introduce classical mechanics in a twofold way, as

solutions to Hamiltonian differential equations and as a theory on a symplectic manifold, respectively. Some results on integrability and Lyapunov theory are also mentioned.

The third chapter is intended as an introduction to quantum mechanics and more particularly to the usual semiclassical theories. A swift review of the Weyl quantization gives way to adequate results in semiclassical propagation. Some results intended for the next chapter on quasi–modes are introduced. Results, mainly focusing on localization, can be found in section 4.4. Adaptations and revision of existing results have been carried out in section 4.5.

Having described general quantum mechanics, we can start with the last chapter which is entirely devoted to a semiclassical characterization of the Wannier–Stark resonances. This involves more general WKB methods with operator valued classical mechanics. Of fear that the involved technicalities might at times become overwhelming, some examples and connections to previous chapters have been introduced. More general results are to be found in sections 5.3.2, 5.3.3. Minor adaptations had to be carried out in section 5.2.2. Results and discussions that are more specific to the Wannier–Stark system are in section 5.4.

Chapter 2

The Hill equation

In this chapter we introduce the theory of Hill operators on Banach spaces in the context of the theory of linear ordinary differential equation (ODE). It further enables us to introduce notation and establish some useful results. For rigorous proofs and a more general introduction to the general theory of linear ODE we refer to, e.g., [Tay96, CL55].

2.1 Initial value problems

We consider an ODE of the form

$$\frac{\mathrm{d}u}{\mathrm{d}t} = f(t, u), \tag{2.1}$$

where u is a continuously differentiable function of the real variable $t \in I \subset \mathbb{R}$ (in the future denoted as $u \in \mathrm{C}^1(I)$). We will call the set of equations

$$\begin{aligned} \frac{\mathrm{d}u}{\mathrm{d}t} &= f(t, u), & (2.2)\\ u(0) &= u_0, & (2.3) \end{aligned}$$

an initial value problem with initial value u_0. In order to state the result of this section, we will need to make the following definitions.

Definition 2.1 (Lipschitz continuity)**.** A continuous function f is said to satisfy a Lipschitz condition on $\mathscr{D} \subset \mathbb{R} \times \mathbb{R}$, if there exists $M \geq 0$ such that $\forall (t, x_1), (t, x_2) \in \mathscr{D}$,

$$|f(t, x_1) - f(t, x_2)| \leq M\,|x_1 - x_2|. \tag{2.4}$$

Furthermore, the constant M will be called Lipschitz constant.

Definition 2.2 (Approximate solution)**.** An $\varepsilon-$approximate solution φ to (2.1) satisfies the following inequality

$$\left|\frac{\mathrm{d}\varphi}{\mathrm{d}t}(t) - f(t, \varphi(t))\right| \leq \varepsilon. \tag{2.5}$$

Theorem 2.1 (Picard-Lindelöf)**.** *If the function $f(t, x)$ is Lipschitz continuous on $\mathscr{D} = (-a, a) \times (-b, b)$ with constant M, then for $|t| < \min\left(a, \frac{b}{M}\right)$ the series*

$$\varphi_{i+1}(t) := u_0 + \int_0^t f\left(\tau, \varphi_i(\tau)\right) \mathrm{d}\tau \tag{2.6}$$

converges uniformly on $\mathscr{D}$ to the unique solution of the initial value problem (2.3).

The concepts used in this proof extend naturally to any Banach space. It is readily verified that the argument holds for vector valued ODE, i.e., ODE on a Banach space $\mathscr{X}$ of the form of (2.1) where $u(t) \in \mathscr{X}$ and $f(t, \bullet)\colon \mathscr{X} \to \mathscr{Y}$.

The uniqueness of solutions enables the construction of unique global solutions on bounded domains.

2.2 Fundamental solutions

A linear ODE $\mathscr{L}(u) = 0$ of order n is endowed with the properties

$$\begin{aligned} \mathscr{L}(u+v) &= \mathscr{L}(u) + \mathscr{L}(v), \\ \mathscr{L}(cu) &= c\mathscr{L}(u), \end{aligned} \tag{2.7}$$

$\forall u, v \in C^{n-1}$, $c \in \mathbb{C}$ and can be written in the form

$$\mathscr{L}(u) = \sum_{i=0}^{n} \alpha_i(t) \frac{\mathrm{d}^i u}{\mathrm{d}t^i}. \tag{2.8}$$

An operation satisfying properties (2.7) will be called linear.

We note that any linear ODE of order n can be brought to a first order vector valued ODE of dimension n. With the choice

$$v_i(t) = u^{(i)}(t), \tag{2.9}$$

where $u^{(i)}$ denotes the ith derivative of u, $\mathscr{L}(u)=0$ amounts to

$$\frac{\mathrm{d}\upsilon_n}{\mathrm{d}t}=-\sum_{i=0}^{n-1}\alpha_i(t)\upsilon_i, \qquad \frac{\mathrm{d}\upsilon_{j+1}}{\mathrm{d}t}=\upsilon_j, \quad \forall j=1,...,n-2,$$

that is

$$\frac{\mathrm{d}U}{\mathrm{d}t}=F(t)U, \qquad U=\left(\upsilon_1,\upsilon_2,...,\upsilon_n\right)^{\mathrm{T}}, \tag{2.10}$$

where T denotes transposition.

Theorem 2.2. *The solutions of $\mathscr{L}(u)=0$ span an $n-$dimensional vector space.*

It follows that any solution can be written as

$$u=\sum_{i=1}^{n}a_i\varphi_i, \tag{2.11}$$

where φ_i are n linearly independent solutions, which in turn implies that the initial value problem

$$\mathscr{L}(u)=0,\ u(0)=u_0,\ \frac{\mathrm{d}}{\mathrm{d}t}u(0)=u_0',...,\frac{\mathrm{d}^{n-1}u(0)}{\mathrm{d}t^{n-1}}=u_0^{(n-1)}, \tag{2.12}$$

can be written as

$$u=X(t)\xi_0, \tag{2.13}$$

where ξ_0 the vector of initial conditions. The matrix $X(t)$ will be defined as the normalized fundamental solution to $\mathscr{L}(u)=0$. More generally, a matrix whose columns are n linearly independent solutions is called a fundamental matrix. The linear independence of solutions can be expressed by the property $\det(X(t))\neq 0$ for a fundamental system X.

We will make use of the following lemmata.

Lemma 2.1 (Grönwall inequality)**.** *Let $u(t)$ satisfy*

$$\frac{\mathrm{d}u}{\mathrm{d}t}=A(t)u. \tag{2.14}$$

Then there exists $C_T>0$ s.t.

$$||u(t)||\leq C_T\mathrm{e}^{\sup_{\tau\in[0,T]}||A(\tau)||t|} \tag{2.15}$$

uniformly on $[0, T]$.

In general, an ODE of the type (2.10) is called homogeneous. This designation is in contrast to inhomogeneous ODE which may contain additional constant terms or functions.

Lemma 2.2 (Duhamel's principle)**.** *Let $X(t)$ be the fundamental matrix of the homogeneous system of linear ODE*

$$\frac{\mathrm{d}u}{\mathrm{d}t} = A(t)u. \tag{2.16}$$

Then

$$u(t) = u_0 + X(t)\int_0^t X^{-1}(\tau)b(\tau)\,\mathrm{d}\tau \tag{2.17}$$

is a solution of the inhomogeneous system of ODE

$$\frac{\mathrm{d}u}{\mathrm{d}t} = A(t)u + b(t) \tag{2.18}$$

with initial value u_0.

We refer to [Tay96] for the proofs.

2.3 Floquet theory

We have now the basic concepts to introduce the main tool to deal with periodic linear ODE, namely the Floquet-Lyapunov theorem, which is also commonly known as the Floquet theorem. At roughly the same time, Floquet [Flo83] and Lyapunov [Lia07] introduced the notion of what is today known as Floquet-solutions to linear periodic ODE. The following theorem is generally attributed to them. We assume here that the linear differential equations are written in the form of (2.10).

Theorem 2.3 (Floquet, Lyapunov)**.** *A linear homogeneous ODE with bounded $\tau-$periodic coefficients has a fundamental solution of the kind*

$$X(t) = \mathrm{e}^{\Lambda t}P(t), \tag{2.19}$$

where Λ is a constant $n \times n$ matrix and P is a $\tau-$periodic bounded matrix valued function.

Proof. We denote by $F(t)$ the bounded $\tau-$periodic $n \times n$ matrix defining the associated first order vector differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}X(t) = F(t)X(t) \tag{2.20}$$

and

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}X(t+\tau) &= F(t+\tau)X(t+\tau) \\ &= F(t)X(t+\tau). \end{aligned} \tag{2.21}$$

Satisfying the same differential equation, $X(t+\tau)$ and $X(t)$ can at most differ by multiplication of a matrix $M \in \mathrm{GL}(n)$,

$$X(t+\tau) = X(t)M = X(t)\mathrm{e}^{\Lambda\tau}, \tag{2.22}$$

since $M \in \mathrm{GL}(n)$. Let further

$$\begin{aligned} P(t) &= X(t)\mathrm{e}^{-\Lambda t} = X(t)\mathrm{e}^{\Lambda\tau}\mathrm{e}^{-\Lambda(t+\tau)} \\ &= P(t+\tau). \end{aligned} \tag{2.23}$$

Then

$$X(t) = \mathrm{e}^{\Lambda t}P(t) \tag{2.24}$$

will have the claimed property. Boundedness of P follows from an application of Grönwall's lemma. Note that the arguments in this proof are "symmetrical" as a similar approach would work as well if we choose to write the Floquet solutions as

$$X(t) = Q(t)\mathrm{e}^{\Pi t}. \tag{2.25}$$

However this does not imply that $\Lambda = \Pi$ and $P = Q$ in general.

□

The Floquet matrix Λ can be brought to block diagonal form with multipliers λ_i. These multipliers will be called Floquet exponents.

2.4 The Hill equation

Hill equations are second order homogeneous differential equations with periodic coefficients. The study of the solutions of Hill equations has attracted a lot of interest over the past 100 years. They appear in astronomy [Hil86, Poi87] and physics [Blo28, Mat68], to name only a few but historically significant examples. There exist numerous reviews on the subject (see, e.g. [MS54, MW66, McL64]).

In general, one considers an equation of the form

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \left(a - \sum_{k=1}^{\infty} a_j \mathrm{e}^{2\mathrm{i}kx}\right)\psi = 0, \tag{2.26}$$

where the periodicity (and boundedness) of the coefficients has been considered. A particularly well-studied example is the Mathieu equation [Mat68]

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + (a - 2q\cos(2x))\psi = 0, \tag{2.27}$$

which is the simplest Hill equation. Of particular importance is the dependence of the Floquet exponents corresponding to (2.26) on the parameter a. In this respect, the treatments of (2.26) and (2.27) do not differ qualitatively. We only consider the Mathieu equation in the $\pi-$periodic case. The general case can be achieved by scaling.

2.4.1 The fundamental system

We seek a Floquet solution to (2.27), i.e., a solution expressed as the function

$$\psi(x) = \mathrm{e}^{\mathrm{i}\lambda x} \sum_{j\in\mathbb{Z}} c_{2j} \mathrm{e}^{2\mathrm{i}jx}, \tag{2.28}$$

where λ is the Floquet exponent of the solution.

Lemma 2.3. *There exists an entire function $\mu(a)$ such that*

$$\cos(\lambda\pi) = \mu(a). \tag{2.29}$$

Proof. The following discussion can be found in [Koh59]. We consider the fundamental system of Floquet solutions ψ_1, ψ_2 generated by the initial conditions

$$\begin{aligned} \psi_1(0) &= 1, \qquad \psi_1'(0) = 0, \\ \psi_2(0) &= 0, \qquad \psi_2'(0) = 1. \end{aligned}$$

A Floquet solution satisfies

$$\psi(x+\pi) = \mathrm{e}^{\mathrm{i}\lambda\pi}\psi(x),$$

hence

$$\begin{aligned} \psi(\pi) &= \mathrm{e}^{\mathrm{i}\lambda\pi}\psi(0), \\ \psi'(\pi) &= \mathrm{e}^{\mathrm{i}\lambda\pi}\psi'(0). \end{aligned}$$

Rewriting $\psi(x)$ as a linear combination of $\psi_1(x)$ and $\psi_2(x)$,

$$\psi = A\psi_1 + B\psi_2, \quad A, B \in \mathbb{C},$$

one obtains the equation

$$e^{2i\lambda\pi} - 2\mu(a)e^{i\lambda\pi} + 1 = 0 \tag{2.30}$$

upon elimination of A and B. Here $\mu(a)$ is a function of a that can be expressed as

$$\mu(a) = \frac{1}{2}\big(\psi_1(\pi; a, q) + \psi_2'(\pi; a, q)\big),$$

where we have have explicitly written the dependence of the functions on the parameters a and q. Multiplication of (2.30) by $e^{-i\lambda\pi}$ gives

$$\cos(\lambda\pi) = \mu(a). \tag{2.31}$$

□

Accordingly, there are two (possibly degenerate) Floquet exponents corresponding to a value of a and it is readily seen that if λ is real we have

$$-1 \leq \quad \lambda(a) \quad \leq 1. \tag{2.32}$$

2.4.2 Hill's determinantal equation

Insertion of the ansatz (2.28) into (2.27) gives the recursion equations

$$c_{2j} + \frac{q}{(2j-\lambda)^2 - a}\big(c_{2(j+1)} + c_{2(j-1)}\big) = 0, \forall j \in \mathbb{Z}. \tag{2.33}$$

We consider this recursion as the system

$$\mathscr{A}\overline{c} = 0 \tag{2.34}$$

of equations, where $\mathscr{A}$ can be considered as an operator on the Hilbert space $\ell^2(\mathbb{Z})$ by virtue of the ansatz, and since $\sum_{j\in\mathbb{Z}} c_{2j}e^{2jx}$ can be seen as a function in $L^2(0, \pi)$.

Proposition 2.1. *$\mathscr{A} - \mathbb{1}$ is a trace class operator on $\ell^2(\mathbb{Z})$.*

Proof. For any $n \in \mathbb{Z}$ we define

$$\mathscr{A}_n(\lambda; a, q) = \begin{pmatrix} 1 & \xi_n & & & & & & & & \\ \xi_{n-1} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \\ & \cdot & \xi_2 & 1 & \xi_2 & 0 & 0 & 0 & \cdot & \\ & \cdot & 0 & \xi_1 & 1 & \xi_1 & 0 & 0 & \cdot & \\ & \cdot & 0 & 0 & \xi_0 & 1 & \xi_0 & 0 & \cdot & \\ & \cdot & 0 & 0 & 0 & \xi_{-1} & 1 & \xi_{-1} & 0 & \cdot \\ & \cdot & 0 & 0 & 0 & 0 & \xi_{-2} & 1 & \xi_{-2} & \cdot \\ & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \xi_{-n+1} \\ & & & & & & & & \xi_{-n} & 1 \end{pmatrix}$$

and

$$\xi_j = \frac{q}{(2j-\lambda)^2 - a}. \tag{2.35}$$

We can consider the operator $\mathscr{B}_n : \mathbb{C}^{2n+1} \to \mathbb{C}^{2n+1}$ with $\mathscr{B}_n := \mathscr{A}_n - \mathbb{1}$. By letting $n \to \infty$, the limiting matrices $\mathscr{A}$, $\mathscr{B}$ will constitute operators on the infinite dimensional Hilbert space $\ell^2(\mathbb{Z})$. Furthermore, $\mathscr{B}$ can be written as

$$\mathscr{B} = \mathscr{B}_{+1} + \mathscr{B}_{-1}, \tag{2.36}$$

where $\mathscr{B}_{+1}$ and $\mathscr{B}_{-1}$ are single sub- and super-diagonal, respectively, with elements $(\ldots, \xi_{-n}, \xi_{-n+1}, \ldots, \xi_{-1}, \xi_0, \xi_1, \ldots)$. The singular values of these operators will hence be $\left|\xi_j\right|$. The sum of the singular values of these operators is

$$\mathrm{tr}\left(\left|\mathscr{B}_{\pm 1}\right|\right) = \sum_{j\in\mathbb{Z}} \left| \frac{q}{(2j-\lambda)^2 - a} \right|, \tag{2.37}$$

which can be rewritten as

$$\sum_{j\in\mathbb{Z}} \left|\xi_j\right| = \frac{1}{4} \sum_{j\in\mathbb{Z}} \left|\frac{1}{j^2}\right| \left| \frac{1}{\left(1 - \frac{\lambda}{2j}\right)^2 - \frac{a}{4j^2}} \right|. \tag{2.38}$$

This sum converges since $\sum_{j\in\mathbb{N}} \frac{1}{j^\chi}$, $\chi > 1$, converges and the terms under the denominator in (2.38) are inferior to $|r|^{-p}$, $1 < p < 2$, for large enough j. This is valid for all finite values of a and λ for which no denominator of ξ_{2j} vanishes, i.e.,

$$2j - \lambda \neq \pm\sqrt{a},\ j \in \mathbb{Z}. \tag{2.39}$$

The operators $\mathscr{B}_{+1}$ and $\mathscr{B}_{-1}$ defined on $\ell^2(\mathbb{Z})$ are therefore trace class operators with trace norms

$$\left\|\mathscr{B}_{\pm 1}\right\|_{\mathrm{tr}} = \mathrm{tr}\left(\left|\mathscr{B}_{\pm 1}\right|\right). \tag{2.40}$$

By the triangle inequality of the trace norm [Kat95] we have

$$\left\| \mathscr{B}_{+1} + \mathscr{B}_{-1} \right\|_{\mathrm{tr}} \;\leq\; \left\| \mathscr{B}_{+1} \right\|_{\mathrm{tr}} + \left\| \mathscr{B}_{-1} \right\|_{\mathrm{tr}}, \tag{2.41}$$

thus

$$\left\| \mathscr{B} \right\|_{\mathrm{tr}} \;\leq\; 2 \left\| \mathscr{B}_{\pm 1} \right\|_{\mathrm{tr}} \;<\; \infty. \tag{2.42}$$

The operator $\mathscr{B}$ is hence also trace class.

□

By the properties of trace class operators [Sim79] one can define the determinant $\det(\mathscr{A}) = \prod_{j\in\mathbb{Z}} \lambda_j(\mathscr{A})$ of the operator $\mathbb{1} + \mathscr{B} = \mathscr{A}$, where $\lambda_j(\mathscr{A})$ are the eigenvalues of $\mathscr{A}$. By the Fredholm alternatives, the operator is then boundedly invertible if and only if $\det(\mathscr{A}) \neq 0$ (see, e.g., [Yaf92]).

2.4.3 The Whittaker-Hill formula

Whittaker was able to produce an astounding formula for the determinant corresponding to the full Hill equation [WW62]. We will describe this result for the determinant $\Delta(a, \lambda) = \det(\mathscr{A}(\lambda; a, q))$ corresponding to the Mathieu problem. We follow McLachlan [McL64].

Proposition 2.2. *$\Delta(a, \lambda)$ is an even, one-periodic function of λ. It is analytic on the strip $0 \leq \mathrm{Re}(\lambda) < 1$ up to simple poles at the values excluded by (2.39).*

Proof. Since j takes all values from $-\infty$ to $+\infty$, the determinant $\Delta(a, \lambda)$ will be left invariant under the change $\lambda \to -\lambda$, hence $\Delta(a, \lambda)$ is even in λ, i.e., $\Delta(a, -\lambda) = \Delta(a, \lambda)$. Furthermore, $(2j - (\lambda + 2)) = (2(j+1) - \lambda)$, giving $\Delta(a, \lambda + 1) = \Delta(a, \lambda)$ again since j takes all values from $-\infty$ to $+\infty$, i.e., the determinant is a periodic function in λ with period 1. Δ is a determinant and thus is a sum of products of $\xi_i(a, \lambda)$. Disregarding their poles, the functions $\xi_i(a, \lambda)$ are analytic functions, hence so is Δ, except at the poles of the functions $\xi_i(a, \lambda)$. We see by the structure of $\mathscr{A}$ that no term in ξ_{2j} will appear in higher powers than one, i.e., all poles are simple and they are given by (2.39).

□

Corollary 2.1. *One can find a function $C(\lambda)$ s.t.*

$$\Theta(a, \lambda) = \Delta(a, \lambda) - C(\lambda) \cdot \mathscr{D}(a, \lambda) \tag{2.43}$$

is independent of the variable $\lambda \in \mathbb{C}$, where

$$\mathscr{D}(a, \lambda) = \frac{1}{\cos(\pi\lambda) - \cos\left(\pi\sqrt{a}\right)}. \tag{2.44}$$

Proof. It is readily seen that the function $\mathscr{D}(a, \lambda)$ also has simple poles at the

poles of $\Delta(a, \lambda)$. $\Delta(a, \lambda)$ has only one pole on the strip $0 \leq \mathrm{Re}(\lambda) < 1$. By the periodicity (in λ) of $\Delta(a, \lambda)$, finding the function $C(\lambda)$ is reduced to calculating the constant $C = C(\lambda)$ corresponding to the quotient between the residues of the functions $\Delta(a, \lambda)$ and $\mathscr{D}(a, \lambda)$ at that pole. With the proper value of C, $\Theta(a, \lambda)$ is analytic in the whole complex plane and has no poles. It must hence, by Liouville's theorem, be a constant. In the limiting case $\lambda \to +i\infty$, the matrix $\mathscr{A}(\lambda; a, q)$ becomes diagonal dominant, i.e., only the diagonal elements (equal to 1) remain in this limit, since $\lim_{\lambda \to i\infty} \xi_{2j} = 0$. Thus

$$\lim_{\lambda \to +i\infty} \Delta(a, \lambda) = 1.$$

We further see that $\lim_{\lambda \to i\infty} \mathscr{D}(a, \lambda) = 0$, hence $\Theta(a, \lambda) = 1$. It follows that

$$C = \frac{\Delta(a, \lambda) - 1}{\mathscr{D}(a, \lambda)}. \tag{2.45}$$

For the case $\lambda = 0$ we have $\mathscr{D}(a, 0) = 1/\left(1 - \cos\left(\pi\sqrt{a}\right)\right)$. Excluding the values of $a = 4j^2$ for which $\Delta(a, \lambda = 0)$ cannot be defined, we can write

$$C = \frac{\Delta(a, 0) - 1}{1 - \cos\left(\pi\sqrt{a}\right)}. \tag{2.46}$$

□

This allows us to conclude this section.

Theorem 2.4 (Whittaker)**.** *We have*

$$\sin^2\left(\frac{\pi\lambda}{2}\right) = \Delta(a, 0)\sin^2\left(\frac{\pi\sqrt{a}}{2}\right), a \neq 4j^2, j \in \mathbb{Z}. \tag{2.47}$$

The formula is found by substitution of (2.46) into (2.45). The characteristic exponents resulting from the eigenvalue a are solutions of this equation. This formula was shown by Whittaker [WW62] for the full Hill problem. The full Hill problem of eq. (2.26) has an infinite number of Fourier coefficients. The matrix $\mathscr{A}$ will in this case be a full matrix, i.e., not merely a tridiagonal matrix as in the Mathieu problem.

2.4.4 An approximation scheme for $\Delta(0, \lambda)$

In many applications, one is dependent on the functions $a(\lambda)$. There exist many schemes to approximate these functions. For a review see, e.g., [MS54, MW66, McL64]). There are also more general consideration for matrix valued Hill

equations; see, e.g., R. Denk [Den95] and predecessors. The latest approximation schemes for the Hill equations that we are aware of can be found in [FP01, Str05]. We here account for the latter. It is an approach based on the Whittaker-Hill formula producing a formula in closed form. The idea is to calculate $\Delta(0, \lambda)$ recursively.

The determinant of an infinite dimensional square matrix can be defined in the Poincaré sense [Poi86], i.e., as the limit of the determinants of finite dimensional matrices. For this purpose, we define the square tridiagonal matrices

$$\mathscr{A}_i^0 = \mathscr{A}_i(\lambda = 0)$$

with diagonal elements 1 and off diagonal elements

$$\left(\xi_{i-1}^0, \xi_{i-2}^0, \ldots, \xi_0^0, \ldots, \xi_{-i}^0\right) \tag{2.48}$$

and

$$\left(\xi_i^0, \ldots, \xi_0^0, \ldots, \xi_{-i+1}^0, \xi_{-i+1}^0\right). \tag{2.49}$$

Here ξ_i^0 denotes $\xi_i(\lambda = 0)$ as previously defined. With this definition we have $\Delta(0)$ as the limiting case of $\Delta_i^0 = \det\left(\mathscr{A}_i^0\right)$, i.e.,

$$\Delta(0) = \lim_{i\to\infty} \Delta_i^0.$$

Since for $\lambda = 0$, $\xi_{-i}^0 = \xi_i^0$, the matrices $\mathscr{A}_i$ are symmetric with respect to the second diagonal.

The matrix $\mathscr{A}_i^0$, $i > 2$, can be written in terms of $\mathscr{A}_{i-1}^0$ through

$$\mathscr{A}_i^0 = \begin{pmatrix} 1 & \xi_i^0 & & & \\ \xi_{i-1}^0 & \cdot & \cdot & \cdot & \\ & \cdot & \mathscr{A}_{i-1}^0 & \cdot & \\ & \cdot & \cdot & \cdot & \xi_{i-1}^0 \\ & & & \xi_i^0 & 1 \end{pmatrix},$$

where the dotted square represent the outer elements of $\mathscr{A}_{i-1}^0$. Defining the truncation operators of a matrix M: $\mathrm{r}(M)$, $\mathrm{l}(M)$, $\mathrm{u}(M)$, $\mathrm{d}(M)$, i.e., the matrices M without left ($\mathrm{r}(M)$), respectively right ($\mathrm{l}(M)$), columns and the upper ($\mathrm{d}(M)$), respectively lower($\mathrm{u}(M)$), rows, we can write the Laplace decomposition of the determinant of the matrix $\mathscr{A}_i^0$. Developing along the first row we get

$$\det\left(\mathscr{A}_i^0\right) = \begin{vmatrix} \cdot & \cdot & \cdot & \\ \cdot & \mathscr{A}_{i-1}^0 & \cdot & \\ \cdot & \cdot & \cdot & \xi_{i-1}^0 \\ & & \xi_i^0 & 1 \end{vmatrix} - \xi_i^0 \begin{vmatrix} \xi_{i-1}^0 & \cdot & \cdot & \cdot & \\ & \cdot & r\left(\mathscr{A}_{i-1}^0\right) & \cdot & \\ & \cdot & \cdot & \cdot & \xi_{i-1}^0 \\ & & & \xi_i^0 & 1 \end{vmatrix},$$

and then developing the first term on the last row and the second term by the first column,

$$\begin{aligned}\det\left(\mathscr{A}_i^0\right) &= \det\left(\mathscr{A}_{i-1}^0\right) - \xi_i^0 \begin{vmatrix} \cdot & \cdot & \cdot & \\ \cdot & \mathrm{l}\left(\mathscr{A}_{i-1}^0\right) & \cdot & \\ \cdot & \cdot & \cdot & \xi_{i-1}^0 \end{vmatrix} \\ &\quad - \xi_i^0\xi_{i-1}^0 \begin{vmatrix} \cdot & \cdot & \cdot & \\ \cdot & \mathrm{dr}\left(\mathscr{A}_{i-1}^0\right) & \cdot & \\ \cdot & \cdot & \cdot & \xi_{i-1}^0 \\ & & \xi_i^0 & 1 \end{vmatrix}.\end{aligned}$$

Proceeding in a similar fashion we can write

$$\begin{aligned}\det\left(\mathscr{A}_i^0\right) &= \Delta_{i-1}^0 - \xi_i^0\xi_{i-1}^0 \det\left(\mathrm{ul}\left(\mathscr{A}_{i-1}^0\right)\right) - \xi_i^0\xi_{i-1}^0 \det\left(\mathrm{rd}\left(\mathscr{A}_{i-1}^0\right)\right) \\ &\quad + \left(\xi_i^0\xi_{i-1}^0\right)^2 \det\left(\mathrm{uldr}\left(\mathscr{A}_{i-1}^0\right)\right).\end{aligned}$$

Clearly, we have $\mathrm{uldr}\left(\mathscr{A}_{i-1}^0\right) = \mathscr{A}_{i-2}^0$. Furthermore, by the symmetry properties around the second diagonal,

$$\det\left(\mathrm{rd}\left(\mathscr{A}_{i-1}^0\right)\right) = \det\left(\mathrm{ul}\left(\mathscr{A}_{i-1}^0\right)\right). \tag{2.50}$$

Thus we conclude that

$$\Delta_i^0 = \Delta_{i-1}^0 - 2\cdot\xi_i^0\xi_{i-1}^0 \det\left(\mathrm{rd}\left(\mathscr{A}_{i-1}^0\right)\right) + \left(\xi_i^0\xi_{i-1}^0\right)^2 \Delta_{i-2}^0. \tag{2.51}$$

By further defining $\Omega_i = \det\left(\mathrm{ul}\left(\mathscr{A}_i^0\right)\right) = \det\left(\mathrm{rd}\left(\mathscr{A}_i^0\right)\right)$ and decomposing by minors, we have

$$\Omega_i = \det\left(\mathscr{A}_{i-1}^0\right) - \xi_i^0\xi_{i-1}^0\Omega_{i-1}. \tag{2.52}$$

Substituting $\det\left(\mathrm{rd}\left(\mathscr{A}_{i-1}^0\right)\right)$ in eq. (2.51) we find the recursion in Δ_i,

$$\Delta_i = \beta_i\Delta_{i-1} - \alpha_i\beta_i\Delta_{i-2} + \alpha_i\alpha_{i-1}^2\Delta_{i-3}, \tag{2.53}$$

where we have substituted $\xi_i^0\xi_{i-1}^0 = \alpha_i$ and $1-\alpha_i = \beta_i$.

Up to now the recursion has been constructed formally. Rewriting (2.51) we remark that

$$\Delta_i^0 - \Delta_{i-1}^0 = \left(\xi_i^0\xi_{i-1}^0\right)^2\Delta_{i-2}^0 - 2\cdot\xi_i^0\xi_{i-1}^0 \det\left(\mathrm{rd}\left(\mathscr{A}_{i-1}^0\right)\right) \tag{2.54}$$

and thus the series can converge ($\lim_{i\to\infty}\xi_i = 0$). In fact, Poincaré himself [Poi86], in his definition of infinite determinants, concluded that this series would converge absolutely if the sum of the non-diagonal elements of $\mathscr{A}^0$ converged absolutely. This is, according to Proposition 2.1, the case here.

2.4.5 A solution to linear recursions without constant terms

Our aim is to write the solutions of Mathieu equation in a completely closed form. To do so we must be able to express the ith term in (2.53), and in particular the limiting term of the series Δ_i^0. We present a method to calculate any term for (in principle) any linear recursion with variable coefficients [Str05]. The important assumption, in addition to the nice behavior of the coefficients, is the fact that constant terms do not occur in the recursions.

The main idea is to be able to construct any term of the series as a sum of all prior terms, i.e., until a sufficient number of consecutive initial values to determine the series. We will assume those to bear the lower indices. Having constructed these sums for the terms, say, $n+1$ and n, a weighted subtraction will render the $(n+1)^{\text{th}}$ term in terms of the initially known ones. For any finite order, the construction makes sense as long as the coefficients are finite. The limiting case, $n \to \infty$, is again to be seen as a formal construction as, in general, one cannot make statements on the convergence of the procedure.

We concentrate on the third order recursion

$$u_i = a_i u_{i-1} + b_i u_{i-2} + c_i u_{i-3}, \tag{2.55}$$

although the procedure could easily be implemented for recursions of any (finite) order. By simply rewriting it for $i-1$ and multiplying it with $-c_i/b_{i-1}$, assuming $b_i \neq 0$, $\forall i$,

$$-\frac{c_i}{b_{i-1}} u_{i-1} = -\frac{a_{i-1}c_i}{b_{i-1}} u_{i-2} - c_i u_{i-3} - \frac{c_i c_{i-1}}{b_{i-1}} u_{i-4}. \tag{2.56}$$

Summing (2.55) and (2.56) one finds

$$u_i = \left(a_i + \frac{c_i}{b_{i-1}}\right) u_{i-1} + \left(b_i - \frac{a_{i-1}c_i}{b_{i-1}}\right) u_{i-2} - \frac{c_i c_{i-1}}{b_{i-1}} u_{i-4}. \tag{2.57}$$

One can hence, by this iteration procedure, construct a sum equal to some u_i over n elements u_k, where the coefficient for u_{i-n+1} vanishes,

$$u_k = \left[\sum_{j=1}^{n-2} \left\{g_n^k\right\}_{k-j} u_{k-j}\right] + \left\{\mathscr{G}_n^k\right\} u_{k-n}. \tag{2.58}$$

Here the $\left\{g_n^k\right\}_{k-j}$ are the coefficients corresponding to the sum equal to u_k with the last term in the sum u_{k-n}. Using this ansatz and eliminating $\left\{\mathscr{G}_n^k\right\} u_{k-n}$ as

previously one finds that

$$\left\{g_{n+1}^k\right\}_{k-j} = \begin{cases} \left\{g_n^k\right\}_{k-j} & , 1 < j \le n-3 \\ \left\{g_n^k\right\}_{k-(n-2)} + \frac{\left\{\mathscr{g}_n^k\right\}}{b_{k-(n-2)}} & , j = n-2 \\ -\left\{\mathscr{g}_n^k\right\} \frac{a_{k-(n-2)}}{b_{k-(n-2)}} \left\{g_n^k\right\}_{k-(n-1)} & , j = n-1 \end{cases},$$

$$\left\{\mathscr{g}_{n+1}^k\right\} = -\left\{\mathscr{g}_n^k\right\} \frac{c_{k-(n-2)}}{b_{k-(n-2)}}.$$

Since these recursions are of first order, one can deduce

$$\left\{g_{n+1}^k\right\}_{k-j} = \begin{cases} \left\{g_n^k\right\}_{k-j} & , 1 < j \le n-3 \\ (-1)^{n-5} \frac{\left\{g_n^k\right\}_{k-(n-2)} c_k c_{k-1}}{b_{k-(n-2)} b_{k-1}} \prod_{j=3}^{n-3} \frac{c_{k-j}}{b_{k-j}} & , j = n-2 \\ (-1)^{n-6} \frac{a_{k-(n-2)} c_k c_{k-1}}{b_{k-(n-2)} b_{k-1}} \prod_{j=3}^{n-3} \frac{c_{k-j}}{b_{k-j}} & , j = n-1 \end{cases},$$

$$\left\{\mathscr{g}_{n+1}^k\right\} = (-1)^{n-5} \frac{c_k c_{k-1}}{b_{k-1}} \prod_{j=3}^{n-3} \frac{c_{k-j}}{b_{k-j}},$$

from the initial values of the recursion given by eq. (2.57). We can hence write all $\left\{g_n^k\right\}_{k-j}$ and $\left\{\mathscr{g}_{n+1}^k\right\}$ explicitly.

Being able to write such sums for any relevant u_k and n, one can eliminate the term of highest index on the r.h.s. of eq. (2.58). If we consider

$$\begin{aligned} u_k &= \left[\sum_{j=1}^{n-2} \left\{g_n^k\right\}_{k-j} u_{k-j}\right] + \left\{\mathscr{g}_n^k\right\} u_{k-n} \\ &= \left\{g_n^k\right\}_{k-1} u_{k-1} + \left[\sum_{j=2}^{n-2} \left\{g_n^k\right\}_{k-j} u_{k-j}\right] + \left\{\mathscr{g}_n^k\right\} u_{k-n} \end{aligned}$$

and

$$u_{k-1} = \left[\sum_{j=1}^{m-2} \left\{g_m^{k-1}\right\}_{k-1-j} u_{k-j}\right] + \left\{\mathscr{g}_m^{k-1}\right\} u_{k-m},$$

summing the two we find

$$\begin{aligned} u_k &= \left[\sum_{j=2}^{n-2}\left\{g_n^k\right\}_{k-j} u_{k-j}\right] + \left\{\mathscr{G}_n^k\right\} u_{k-n} \\ &\quad + \left\{g_n^k\right\}_{k-1}\left[\sum_{j=2}^{m-1}\left\{g_m^{k-1}\right\}_{k-j} u_{k-j}\right] + \left\{g_n^k\right\}_{k-1}\left\{\mathscr{G}_m^{k-1}\right\} u_{k-1-m}. \end{aligned}$$

If we choose m such that

$$m+1=n,$$

we find

$$\begin{aligned} u_k &= \left(\left\{g_n^k\right\}_{k-2} + \left\{g_n^k\right\}_{k-1}\left\{g_{n-1}^{k-1}\right\}_{k-2}\right) u_{k-2} \\ &\quad + \left[\sum_{j=3}^{n-2}\left(\left\{g_n^k\right\}_{k-j} + \left\{g_n^k\right\}_{k-1}\left\{g_{n-1}^{k-1}\right\}_{k-j}\right) u_{k-j}\right] \\ &\quad + \left(\left\{\mathscr{G}_n^k\right\} + \left\{g_n^k\right\}_{k-1}\left\{\mathscr{G}_{n-1}^{k-1}\right\}\right) u_{k-n}. \end{aligned} \tag{2.59}$$

Upon ℓ such eliminations, one can hence write u_k as

$$u_k = \sum_{j=\ell+1}^{n-2}\left\{\gamma_n^k\right\}_{k-j}^{\ell} u_{k-j} + \left\{\Gamma_n^k\right\}^{\ell} u_{k-n} \tag{2.60}$$

where $\left\{\gamma_n^k\right\}_{k-j}^{\ell}$ and $\left\{\Gamma_n^k\right\}^{\ell}$ are the coefficients corresponding to u_{k-j} and u_{k-n} respectively, after ℓ eliminations. If we proceed as previously and eliminate $u_{k-(\ell+1)}$, we get

$$\begin{aligned} u_k &= \sum_{j=\ell+2}^{n-2}\left(\left\{\gamma_n^k\right\}_{k-j}^{\ell} + \left\{\gamma_n^k\right\}_{k-\ell-1}^{\ell}\left\{g_{n-\ell}^{k-\ell}\right\}_{k-j}\right) u_{k-j} \\ &\quad + \left(\left\{\gamma_n^k\right\}_{k-\ell-1}^{\ell}\left\{\mathscr{G}_{n-\ell}^{k-\ell}\right\} + \left\{\Gamma_n^k\right\}^{\ell}\right) u_{k-n}. \end{aligned}$$

Thus we can define recursions for $\left\{\gamma_n^k\right\}_{k-j}^{\ell}$ and $\left\{\Gamma_n^k\right\}^{\ell}$ through

$$\begin{aligned} \left\{\gamma_n^k\right\}_{k-j}^{\ell+1} &= \left\{\gamma_n^k\right\}_{k-j}^{\ell} + \left\{\gamma_n^k\right\}_{k-\ell-1}^{\ell}\left\{g_{n-\ell}^{k-\ell}\right\}_{k-j}, \\ \left\{\Gamma_n^k\right\}^{\ell+1} &= \left\{\gamma_n^k\right\}_{k-\ell-1}^{\ell}\left\{\mathscr{G}_{n-\ell}^{k-\ell}\right\} + \left\{\Gamma_n^k\right\}^{\ell}, \end{aligned} \tag{2.61}$$

which are second, respectively first, order recursions.

By calculating the coefficient of u_{k-j} of highest index, i.e., $\left\{\gamma_n^k\right\}_{k-\ell-1}^{\ell}$, one can recognize a structure for these coefficients. Thus $\left\{\gamma_n^k\right\}_{k-\ell-1}^{\ell}$ can be written as a sum of products of $\left\{g_{n-\mu}^{k-\mu}\right\}_{k-\lambda}$, where the number of terms in the products ranges over all values from 1 to $\ell+1$. As an example, we consider such a sum for $\left\{\gamma_n^k\right\}_{k-7}^{6}$ for terms with four factors of $\left\{g_{n-\mu}^{k-\mu}\right\}_{k-\lambda}$. These terms are written in the left column and the indices (μ, λ) corresponding to the terms $\left\{g_{n-\mu}^{k-\mu}\right\}_{k-\lambda}$ are shown in the right column (Table 2.1),

One can construct the sequences of indices (μ, λ) by considering a line with $\ell+1$ points labeled in ascending order from 0 to ℓ. By further considering p unidirectional non-stationary jumps from the point labeled 0 to the point labeled ℓ, one gets a sequence of initial and final points for the jumps, e.g., $\{(0,1)(1,2)(2,4)(4,6)\}$ for $\ell=6$ and $p=4$. We define the ensemble $\mathscr{S}_p^{\ell+1}$ of all such possible jumps, and by $\left\{\mathscr{S}_p^{\ell+1}\right\}_i$ its ith element. We can hence write the sum of all terms with p factors in $\left\{g_{n-\mu}^{k-\mu}\right\}_{k-\lambda}$ as

$$\mathscr{P}_p^{\ell+1} = \sum_i \prod_{(\mu,\lambda)\in\left\{\mathscr{S}_p^{\ell+1}\right\}_i} \left\{g_{n-\mu}^{k-\mu}\right\}_{k-\lambda}, \tag{2.62}$$

whereupon we find

$$\begin{aligned} \left\{\gamma_n^k\right\}_{k-m-1}^{\ell} &= \sum_{p=1}^{\ell+1} \mathscr{P}_p^{\ell+1} \\ &= \sum_{p=1}^{\ell+1} \sum_i \prod_{(\mu,\lambda)\in\left\{\mathscr{S}_p^{\ell+1}\right\}_i} \left\{g_{n-\mu}^{k-\mu}\right\}_{k-\lambda}. \end{aligned} \tag{2.63}$$

With this, we can simply write the now first order recursions (2.61) as

$$\begin{aligned} \left\{\gamma_n^k\right\}_{k-j}^{\ell+1} &= \left\{g_n^k\right\}_{k-j} + \sum_{\sigma=0}^{\ell} \left\{\gamma_n^k\right\}_{k-m-1}^{\sigma} \left\{g_{n-\sigma-1}^{k-\sigma-1}\right\}_{k-j}, \\ \left\{\Gamma_n^k\right\}^{\ell+1} &= \left\{\mathscr{G}_n^k\right\} + \sum_{\sigma=0}^{\ell} \left\{\gamma_n^k\right\}_{k-m-1}^{\sigma} \left\{\mathscr{G}_{n-\sigma-1}^{k-\sigma-1}\right\}, \end{aligned} \tag{2.64}$$

$$
\begin{aligned}
&\left\{g_n^k\right\}_{k-1}\left\{g_{n-1}^{k-1}\right\}_{k-2}\left\{g_{n-2}^{k-2}\right\}_{k-3}\left\{g_{n-3}^{k-3}\right\}_{k-6}+ \;\vdots\; (0,1)(1,2)(2,3)(3,6)\\
&+\left\{g_n^k\right\}_{k-1}\left\{g_{n-1}^{k-1}\right\}_{k-2}\left\{g_{n-2}^{k-2}\right\}_{k-4}\left\{g_{n-4}^{k-4}\right\}_{k-6}+ \;\vdots\; (0,1)(1,2)(2,4)(4,6)\\
&+\left\{g_n^k\right\}_{k-1}\left\{g_{n-1}^{k-1}\right\}_{k-2}\left\{g_{n-2}^{k-2}\right\}_{k-5}\left\{g_{n-5}^{k-5}\right\}_{k-6}+ \;\vdots\; (0,1)(1,2)(2,5)(5,6)\\
&+\left\{g_n^k\right\}_{k-1}\left\{g_{n-1}^{k-1}\right\}_{k-3}\left\{g_{n-3}^{k-3}\right\}_{k-4}\left\{g_{n-4}^{k-4}\right\}_{k-6}+ \;\vdots\; (0,1)(1,3)(3,4)(4,6)\\
&+\left\{g_n^k\right\}_{k-1}\left\{g_{n-1}^{k-1}\right\}_{k-3}\left\{g_{n-3}^{k-3}\right\}_{k-5}\left\{g_{n-5}^{k-5}\right\}_{k-6}+ \;\vdots\; (0,1)(1,3)(3,5)(5,6)\\
&+\left\{g_n^k\right\}_{k-1}\left\{g_{n-1}^{k-1}\right\}_{k-4}\left\{g_{n-4}^{k-4}\right\}_{k-5}\left\{g_{n-5}^{k-5}\right\}_{k-6}+ \;\vdots\; (0,1)(1,4)(4,5)(5,6)\\
&+\left\{g_n^k\right\}_{k-2}\left\{g_{n-2}^{k-2}\right\}_{k-3}\left\{g_{n-3}^{k-3}\right\}_{k-4}\left\{g_{n-4}^{k-4}\right\}_{k-6}+ \;\vdots\; (0,2)(2,3)(3,4)(4,6)\\
&+\left\{g_n^k\right\}_{k-2}\left\{g_{n-2}^{k-2}\right\}_{k-3}\left\{g_{n-3}^{k-3}\right\}_{k-5}\left\{g_{n-5}^{k-5}\right\}_{k-6}+ \;\vdots\; (0,2)(2,3)(3,5)(5,6)\\
&+\left\{g_n^k\right\}_{k-2}\left\{g_{n-2}^{k-2}\right\}_{k-4}\left\{g_{n-4}^{k-4}\right\}_{k-5}\left\{g_{n-5}^{k-5}\right\}_{k-6}+ \;\vdots\; (0,2)(2,4)(4,5)(5,6)\\
&+\left\{g_n^k\right\}_{k-3}\left\{g_{n-3}^{k-3}\right\}_{k-4}\left\{g_{n-4}^{k-4}\right\}_{k-5}\left\{g_{n-5}^{k-5}\right\}_{k-6} \;\vdots\; (0,3)(3,4)(4,5)(5,6).
\end{aligned}
$$

Table 2.1: $\left\{\gamma_n^k\right\}_{k-7}^{6}$ for terms with four $\left\{g_{n-\mu}^{k-\mu}\right\}_{k-\lambda}$ factors. These terms are written in the left column and the indices (μ, λ) (right column) corresponding to the terms $\left\{g_{n-\mu}^{k-\mu}\right\}_{k-\lambda}$ (left column).

or using the properties of $\left\{\gamma_n^k\right\}_{k-m-1}^{\ell}$,

$$\begin{aligned}\left\{\gamma_n^k\right\}_{k-j}^{\ell+1} &= \left\{g_n^k\right\}_{k-j} + \sum_{\sigma=0}^{\ell}\left[\sum_{p=1}^{\sigma+1}\mathscr{P}_p^{\ell+1}\right]\left\{g_{n-\sigma-1}^{k-\sigma-1}\right\}_{k-j}, \qquad (2.65)\\ \left\{\Gamma_n^k\right\}^{\ell+1} &= \left\{\mathscr{G}_n^k\right\} + \sum_{\sigma=0}^{\ell}\left[\sum_{p=1}^{\sigma+1}\mathscr{P}_p^{\ell+1}\right]\left\{\mathscr{G}_{n-\sigma-1}^{k-\sigma-1}\right\}.\end{aligned}$$

The elimination process can be iterated until only three terms remain in

$$\begin{aligned}u_k &= \sum_{j=n-3}^{n-2}\left\{\gamma_n^k\right\}_{k-j}^{n-4} u_{k-j} + \left\{\Gamma_n^k\right\}^{n-4} u_{k-n} \qquad (2.66)\\ &= \left\{\gamma_n^k\right\}_{k-n-3}^{n-4} u_{k-n-3} + \left\{\gamma_n^k\right\}_{k-n-2}^{n-3} u_{k-n-2} + \left\{\Gamma_n^k\right\}^{n-4} u_{k-n}.\end{aligned}$$

Here, $\left\{\gamma_n^k\right\}_{k-n-3}^{n-4}$, $\left\{\gamma_n^k\right\}_{k-n-2}^{n-3}$ and $\left\{\Gamma_n^k\right\}^{n-4}$ can be calculated explicitly with the help of $\left\{g_{n-\mu}^{k-\mu}\right\}_{k-\lambda}$. Since $\left\{g_{n-\mu}^{k-\mu}\right\}_{k-\lambda}$ are also known explicitly, eq. (2.66) is an explicit solution for u_k knowing u_{k-n-3}, u_{k-n-2} and u_{k-n} for some relevant n.

The only assumption we have made here is that $b_i \neq 0$, $\forall i$.

2.4.6 The Whittaker-Formula in a closed form

Using the results of section 2.4.5, equation (2.53) can be written

$$\Delta_k = \left\{\gamma_n^k\right\}_{k-n-3}^{n-4}\Delta_{k-n-3} + \left\{\gamma_n^k\right\}_{k-n-2}^{n-3}\Delta_{k-n-2} + \left\{\Gamma_n^k\right\}^{n-4}\Delta_{k-n} \qquad (2.67)$$

with

$$\begin{aligned}\left\{\gamma_n^k\right\}_{k-j}^{\ell+1} &= \left\{g_n^k\right\}_{k-j} + \sum_{\sigma=0}^{\ell}\left[\sum_{p=1}^{\sigma+1}\mathscr{P}_p^{\ell+1}\right]\left\{g_{n-\sigma-1}^{k-\sigma-1}\right\}_{k-j}, \qquad (2.68)\\ \left\{\Gamma_n^k\right\}^{\ell+1} &= \left\{\mathscr{G}_n^k\right\} + \sum_{\sigma=0}^{\ell}\left[\sum_{p=1}^{\sigma+1}\mathscr{P}_p^{\ell+1}\right]\left\{\mathscr{G}_{n-\sigma-1}^{k-\sigma-1}\right\}.\end{aligned}$$

Using the properties of the coefficients of (2.53),

$$\left\{g^k_{n+1}\right\}_{k-j} = \begin{cases} \left\{g^k_n\right\}_{k-j}, & 1<j\leq n-3 \\ (-1)^{n-5}\left\{g^k_n\right\}_{k-(n-2)}\times & \\ \quad\times\frac{\alpha_k\alpha^3_{k-1}\alpha^2_{k-2}}{\beta_{k-(n-2)}\beta_{k-1}}\prod_{j=3}^{n-3}\frac{\alpha^2_{k-j-1}}{\beta_{k-j}}, & j=n-2 \\ (-1)^{n-6}\frac{\alpha_k\alpha^2_{k-1}\alpha^2_{k-2}}{\alpha_{k-(n-2)}\beta_{k-1}}\times & \\ \quad\times\prod_{j=3}^{n-3}\frac{\alpha^2_{k-j-1}}{\beta_{k-j}}, & j=n-1 \end{cases}, \quad (2.69)$$

$$\left\{\mathcal{G}^k_{n+1}\right\} = (-1)^{n-5}\frac{\alpha_k\alpha^2_{k-1}\alpha^2_{k-2}}{\beta_{k-1}}\prod_{j=3}^{n-3}\frac{\alpha^2_{k-j-1}}{\beta_{k-j}}. \quad (2.70)$$

We have thus found an explicit expression for $\Delta(0)$. Note that the denominators diverge for those values of a for which $\beta_i = 1-\alpha_i = 0$.

Unfortunately, the form of eq. (2.67) does not, à priori, shed light on specific properties of the solutions of the Whittaker-Hill formula eq. (2.47). Such constructions do, however, have numerical applications [FP01, Den95, Str08].

2.5 Asymptotic behavior and Lyapunov stability

We have above described the construction of solutions in $C^2(\mathbb{R})$ by continuation of the Fourier ansatz of (2.28). Note that one can readily make an important differentiation as to the asymptotic behavior of

$$\psi(x) = e^{i\lambda x}P(x). \quad (2.71)$$

If the imaginary part of $\lambda(a)$ does not vanish, the corresponding Floquet solution will not be bounded in x. Recall that by the Floquet-Lyapunov theorem, $P(x)$ is a bounded function and will hence not contribute to the growth of the function. This observation will be important in our future considerations. The values of a delimit regions where Floquet solutions are either stable or unstable depending on the corresponding Floquet exponent. This phenomenon was already recognized by Lyapunov [Lia07]. This is clear when considering (2.31) with real a. The critically stable solutions are given by the degenerate case, i.e., when both possible Floquet exponents coincide, corresponding to the case

$$\mu(a) = \pm 1 \quad (2.72)$$

in (2.29). The occurrence and the number of such intervals, however, depends on the particularities of the considered periodic coefficients.

The concept of stability will in this thesis play an important role. The term stability (or instability) of motion is strongly associated with the work of Lyapunov [Lia07].

We refer here to ODEs of the form (2.1).

Definition 2.3 (Lyapunov exponent)**.** Let u be solution of (2.1). The smallest positive real number γ satisfying

$$\exists C > 0 \quad \text{s.t.} \quad ||u(t)||\mathrm{e}^{-\gamma|t|} \leq C \tag{2.73}$$

is called the Lyapunov or characteristic exponent of u.

This naturally leads to a very special case.

Definition 2.4 (Lyapunov asymptotic stability)**.** A solution to (2.1) with vanishing Lyapunov exponent is called asymptotically stable.

Hence, such solutions grow slower than any exponential as $|t| \to \infty$. Generally $\gamma \neq 0$ in which case, the solution will be called asymptotically unstable.

Note that if f is Lipschitz continuous with constant M, one has automatically the existence of a constant $C > 0$ such that

$$||u|| \leq C\mathrm{e}^{M|t|}, \tag{2.74}$$

implying one of the two cases above, i.e., Lyapunov asymptotic stability or instability. In such a case, we will generally speak of regular motion in the asymptotically stable case. It is readily seen that the exponentially unstable case will be the generic one. It will also be called chaotic.

Chapter 3

Classical mechanics

Along this thesis, we will encounter non-relativistic classical mechanics. Classical mechanics effectively describe physical systems when quantum (and relativistic) effects can be neglected. Relativistic effects remain small if the velocities of the particles can be considered small in relation to the speed of light. Quantum effects remain small if the typical scale of the system is much larger than the deBroglie wavelength of the particles. We introduce the basic structures. In analogy to the last section, we introduce stability of trajectories. We also introduce the concept of integrability, which will play a particular role further on. For further references and proofs we refer to [Arn78, AM78, Gol80].

3.1 Structures of classical mechanics

We will restrict our considerations to Hamiltonian mechanics of point particles. A classical system is exhaustively described by the set of $2d$ coordinates $X = (p, q)$. The set $\mathscr{P}$ of possible values (p, q) of the system is called phase space. The configuration variable, e.g., position in space, is usually q, and p usually denotes the momentum. The description of the system is then given by an energy function $H : \mathscr{P} \to \mathbb{R}$. H generates integral curves $\Phi^t_H(X_0) = \big(p_t(p_0, q_0), q_t(p_0, q_0)\big)$ according to Hamilton's equation of motion

$$\frac{\mathrm{d}\Phi^t_H(X_0)}{\mathrm{d}t} = \mathscr{J} H'\Big(\Phi^t_H(X_0)\Big).$$

H' denotes the gradient of H and $\mathscr{J}$ is the symplectic unity, that is

$$\mathscr{J} := \begin{pmatrix} 0 & -\mathbb{1}_{d\times d} \\ \mathbb{1}_{d\times d} & 0 \end{pmatrix}.$$

X_0 denotes the initial value.

We will assume that $H(X)$ will be equal to a constant energy E along a trajectory. Observables, i.e., measurable quantities $A : \mathscr{P} \times \mathbb{R} \to \mathbb{R}$ will then follow the equation of motion

$$\frac{\mathrm{d}A_t}{\mathrm{d}t} = \{H, A_t\}_{(p,q)} + \frac{\partial A_t}{\partial t}, \tag{3.1}$$

where

$$\{f, g\}_{(p,q)} = \frac{\partial f}{\partial p}\frac{\partial g}{\partial q} - \frac{\partial f}{\partial q}\frac{\partial g}{\partial p} \tag{3.2}$$

is the Poisson bracket.

The mathematical structure described above can be reformulated if one identifies the phase space $\mathscr{P}$ with a cotangent bundle T^*M where M is assumed to be a smooth manifold describing configuration space. Actually, T^*M is a symplectic manifold with non degenerate symplectic form ω.

Theorem 3.1. *The Hamiltonian flow Φ_H^t generated by a Hamiltonian*

$$H : \mathrm{T}^*M \to \mathbb{R} \tag{3.3}$$

is a symplectomorphism.

This means amongst others that the Hamiltonian flow is a volume preserving transformation. Symplectomorphisms are also called canonical transformations.

3.2 Stability of trajectories

The stability of trajectories will play an important role further on. We adapt here the concepts of Lyapunov stability to classical trajectories. The study of this stability is closely related to the properties of the symplectic matrices (see appendix A).

Proposition 3.1. *The differential of a symplectomorphism is a symplectic matrix.*

Since the flow differential is a map $\mathrm{D}\Phi_H^t : \mathrm{T}_X M \to \mathrm{T}_{X'} M$, one considers the map $\mathrm{D}\Phi_H^t{}^* \circ \mathrm{D}\Phi_H^t : \mathrm{T}_X M \to \mathrm{T}_X M$ to define the Lyapunov exponents of a classical trajectory in analogy to (2.73).

Definition 3.1 (Lyapunov exponents of a classical trajectory)**.** The Lyapunov exponents γ_i of a classical trajectory $\Phi_H^t(X_0)$ are

$$\gamma_i = \lim_{t\to\infty} \sup \left(\frac{\ln\left(s_i\left(\mathrm{D}\Phi_H^t(X_0)\right)\right)}{t} \right), \tag{3.4}$$

where the $s_i\left(\mathrm{D}\Phi_H^t(X_0)\right)$ are the singular values of the flow differential.

When the index i is omitted or the distinction is clear, *the Lyapunov exponent of a classical trajectory* $\Phi_H^t(X_0)$ will denote the maximal Lyapunov exponent, i.e.,

$$\gamma = \max_i\{\gamma_i\}. \tag{3.5}$$

In analogy to solutions to linear ODE, one can discriminate two major types of behavior.

Definition 3.2 (Stable classical motion)**.** A trajectory with Lyapunov exponent zero will be called stable.

Definition 3.3 (Unstable classical motion)**.** A trajectory with non-vanishing Lyapunov exponent will be called chaotic.

One notes that generally there are singular values of s_i less than one. Such singular values correspond to directions in a plane perpendicular to the trajectory where two neighboring trajectories will tend to converge. Since then $\frac{1}{s_i}$ is also a singular value (see appendix A), there will be a corresponding direction where two neighboring trajectories will tend to diverge, thus ensuring volume conservation both globally and locally. Moreover, two singular values are always equal to 1. These correspond to the direction of the Hamiltonian vector field and to the direction perpendicularly to the energy shell, respectively. The energy shell Ω_E denotes the level set defined by $\{X \in \mathrm{T}^*M : H(X) = E\}$.

It follows from the definition of the Lyapunov exponents that the Hilbert-Schmidt norm of the Flow differential will have exponential or polynomial bound in time if the motion is chaotic or stable, respectively. Furthermore, the Hamiltonian equations of motion imply

$$\begin{aligned} \frac{\mathrm{d}S_t}{\mathrm{d}t} &= \mathscr{J}H''(X_t)S_t, \\ S_0 &= \mathbb{1}_{2d\times 2d}, \end{aligned} \tag{3.6}$$

where we have switched to the shorthand S_t for the flow differential $\mathrm{D}\Phi_H^t$, a notation that we will frequently use below.

3.3 Hamilton-Jacobi theory

Given a classical system, one could ask if it is possible to generate coordinates in which the description of this system would be particularly simple. The method of Hamilton-Jacobi does just this. It produces a symplectomorphism, also called a canonical transformation in the context of classical mechanics, which maps the coordinates such that the new momenta α_i are constant. We recall that canonical coordinates p and q satisfy

$$\{p, q\} \stackrel{\text{def}}{=} 1 \tag{3.7}$$

and that canonical transformations (symplectomorphisms) conserve this relation (hence the name canonical). Such a symplectomorphism is specified by a generating function $\mathsf{S}(q, \alpha, t)$. Generally, original or transformed coordinates can be generated by partial derivation by the original/transformed coordinates of this function. In this particular case, S generates the original momentum p by

$$p_i = \frac{\partial \mathsf{S}(q, \alpha, t)}{\partial q_i}. \tag{3.8}$$

The canonical coordinate corresponding to α_i is given by

$$\theta_i = \frac{\partial \mathsf{S}(q, \alpha, t)}{\partial \alpha_i}. \tag{3.9}$$

Theorem 3.2. *Let $H \in \mathrm{C}^\infty(\mathrm{T}^*M)$ be a time independent Hamilton function. Then the Hamilton-Jacobi system is described by the transformation given by the function*

$$\mathsf{S}(q, \alpha, t) = \int p(q, \alpha)\,\mathrm{d}q - Et \tag{3.10}$$

which satisfies the Hamilton-Jacobi equation

$$H\left(\frac{\partial \mathsf{S}(q, \alpha, t)}{\partial q_i}, q\right) - \frac{\partial \mathsf{S}(q, \alpha, t)}{\partial t} = 0. \tag{3.11}$$

The integral

$$\mathscr{S} = \int p(q, \alpha, t)\,\mathrm{d}q \tag{3.12}$$

is called the reduced action. We note that it satisfies

$$H\left(\frac{\partial \mathscr{S}}{\partial q_i}, q\right) = E. \tag{3.13}$$

Since the energy is a constant of the motion, α can be identified such that the reduced action is a function of the type $\mathscr{S}(q, E)$ in one dimension.

For further reference, we will need some properties of Lagrangian manifolds.

Definition 3.4 (Lagrangian manifold)**.** A submanifold Λ of a symplectic manifold is a Lagrangian manifold if

- $\dim(\Lambda) = d$,
- the symplectic form vanishes on Λ.

Lemma 3.1. *Let $S \in \mathrm{C}^\infty(M)$ generate*

$$\Lambda_S = \{(p, q) \in \mathrm{T}^*M : \; p = \nabla_q S\}. \tag{3.14}$$

Then, Λ_S is a Lagrangian manifold. Conversely, any Lagrangian submanifold is locally generated by some function $S \in \mathrm{C}^\infty(M)$.

The last lemma will be useful in locally parameterizing classical trajectories. Two choices will be of use later. Locally, i.e. in a neighborhood, one can choose the coordinates $\left(\nabla_q S, q\right)$ and $\left(p, \nabla_p S\right)$ along a trajectory.

3.4 Periodic structures of integrability

We introduce here a characterization of integrability[1] which is due to Arnold [Arn78] and Liouville [Lio55].

Theorem 3.3 (Liouville, Arnold [Arn78])**.** *Suppose that we are given d functions $A_i \in \mathrm{C}^\infty(\mathrm{T}^*M)$ $(A_1 = H)$ on a $2d$-dimensional cotangent bundle T^*M satisfying*

$$\{A_i, A_j\} = 0. \tag{3.15}$$

Consider the level sets of these functions

$$M_\alpha = \{X \in \mathrm{T}^*M : A_i = \alpha_i\}, \quad \alpha = \{\alpha_1, \alpha_2, ..., \alpha_d\}. \tag{3.16}$$

Assume the d functions are independent (i.e., the d one forms $\mathrm{d}A_i$ are linearly independent at each point of M_α). Then:

[1] For considerations as to the stability of integrable motion we refer to [Laz93] (see KAM tori).

1. *M_α is a smooth manifold, invariant under the phase flow with Hamiltonian H.*

2. *If the manifold M_α is compact and connected, then it is diffeomorphic to a $d-$dimensional torus*

$$\mathbb{T}^d \cong \{(\varphi_1, \varphi_2, ..., \varphi_d) \bmod 2\pi\}. \tag{3.17}$$

3. *The flow generated by H determines a conditionally periodic motion on M_α, i.e., in angular coordinates $\varphi = (\varphi_1, \varphi_2, ..., \varphi_d)$ we have*

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = \omega, \quad \omega = \omega(\alpha). \tag{3.18}$$

4. *Hamilton's equations of motion can be integrated by quadratures.*

The fact that integrable motion is diffeomorphic to linear motion on a $d-$torus implies that it is quasi-periodic. We also note that the action–angle coordinates $(\mathscr{I}, \varphi)$ on a Liouville–Arnold torus are given by the invariants

$$\mathscr{I}_i = \frac{1}{2\pi} \oint_{\mathscr{C}_i} p \, \mathrm{d}q \tag{3.19}$$

where $\mathscr{C}_i$ is the cycle described by the ith linear motion and φ_i its canonical conjugate. The symplectomorphism transforming the system to the Liouville–Arnold system is of the same type as $\mathsf{S}(q, \alpha, t)$ and is generated by a function of the form $\mathscr{S}(q, \mathscr{I})$.

Chapter 4

Quantum mechanics

The aim of this chapter is to introduce quantum mechanics in an appropriate way for us. This will be considered in its non-relativistic formulation. Our approach will be fairly straightforward.

The basic objects of quantum mechanics are observables, states and a set of postulates which set the physical theory. The states usually are vectors in a Hilbert space. The observables form an algebra of self-adjoint operators on that space. There exist several interpretations of quantum mechanics.

The typical model is the self-adjoint operators on the separable Hilbert space $\mathrm{L}^2\left(\mathbb{R}^d\right)$ with the canonical inner product. Physically measurable quantities are given by the spectrum of self-adjoint operators $\widehat{A}$. The expectation of an observable $\widehat{A}$ when the system is in the state ψ is given by inner product

$$\left\langle \psi | \widehat{A}\psi \right\rangle, \psi \in \mathrm{L}^2\left(\mathbb{R}^d\right), ||\psi||_{\mathrm{L}^2\left(\mathbb{R}^d\right)} = 1. \tag{4.1}$$

All normalized states in $\mathrm{L}^2\left(\mathbb{R}^d\right)$ are à priori allowed. Self–adjointness ensures that real values are obtained. The states are normalized $\langle \psi | \psi \rangle = 1$ such that $\psi^* \psi$ is a positive normalized measure on $\mathbb{R}^d$ seen as the position probability density of the particle. Note that by the definition of the expectation value (4.1) we need only consider states modulo some phase $\mathrm{e}^{\mathrm{i}\alpha}$, $\alpha \in \mathbb{R}$, i.e., we actually consider the projective Hilbert space of $\mathrm{L}^2\left(\mathbb{R}^d\right)$.

The dynamics is dictated by a strongly continuous one parameter group of operators $\mathscr{U}(t)$ generated by an essentially self-adjoint operator[1] $\widehat{H}$, the Hamilton operator, densely defined on $\mathrm{L}^2\left(\mathbb{R}^d\right)$. Typically, the Hamilton operator will

[1]With some nonchalance, we will, mostly, not make any distinction between an essentially self–adjoint operator and its self-adjoint extension since, in our case, there do not reside any ambiguities.

be of the form of a Schrödinger operator, i.e.,

$$\widehat{H} = -\hbar^2 \triangle + V(x). \tag{4.2}$$

We wish to introduce such a theory using the Weyl quantization.

4.1 Pseudo–differential operators

We will here introduce the Weyl quantization scheme. The construction can be seen as a realization of linear operators on $\mathrm{L}^2\left(\mathbb{R}^d\right)$ as pseudo–differential operators (ΨDO). Identifying the momentum operator as the gradient and the position operator as the multiplication by x, i.e.,

$$\widehat{x} = x \tag{4.3}$$
$$\widehat{p} = -\mathrm{i}\hbar\partial_x, \tag{4.4}$$

these are essentially self-adjoint operators on appropriate domains generating the strongly continuous operators $\widehat{\mathscr{T}}(p,q) = \exp\left(\frac{\mathrm{i}}{\hbar}\left(p\widehat{x} - q\widehat{p}\right)\right)$ on $\mathrm{L}^2\left(\mathbb{R}^d\right)$. These operators induce a shift in p and q in the momentum, respectively position, representation of a function $\psi \in \mathrm{L}^2\left(\mathbb{R}^d\right)$, i.e.,

$$\widehat{\mathscr{T}}(p,q)\psi(x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p\left(x-\frac{q}{2}\right)}\psi(x-q). \tag{4.5}$$

With this in mind it is possible to construct operators associated to functions on $\mathbb{R}^{2d}$ (see, e.g. [Fol89, Rob87]). More specifically, the Weyl quantization of a smooth function h, a symbol, is given by the following integral,

$$\mathrm{Op}^{\mathrm{w}}_{\hbar}[h]\,\psi = \frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^{2d}} h\left(\frac{x+y}{2},\,\xi\right)\psi(y)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x-y)\xi}\,\mathrm{d}y\mathrm{d}\xi\,. \tag{4.6}$$

We also wish to construct operators from a suitable class of operator valued symbols. The construction does not differ substantially from the scalar case, thus we present the more general setting directly. Our main sources are [DS99, Fol89] and references therein. We here consider smooth functions on $\mathbb{R}^{2d}$ into the algebra of bounded operators on a separable[2] Hilbert space $\mathscr{H}_0$ that decrease faster than any polynomial, i.e., the Schwartz space of $\mathscr{B}(\mathscr{H}_0)$-valued functions on $\mathbb{R}^{2d}$, $\mathcal{S}\left(\mathbb{R}^{2d}, \mathscr{B}(\mathscr{H}_0)\right)$. As a cautionary note, we wish to forewarn that we will encounter quantizations in other parameters than $\hbar$ later in this thesis[3].

[2] We only encounter separable Hilbert spaces in this thesis. Any mentioned Hilbert space will, form this point on, be assumed separable.

[3] This generates a somewhat cumbersome but necessary notation.

We recall that a Bochner integral takes values in Banach spaces and is defined analogously to a Lebesgue integral.

Definition 4.1 (Symbol class)**.** The operator valued functions of the symbol class $S^k_m\left(\mathbb{R}^{2d}, \mathscr{B}(\mathscr{H}_0)\right)$ are the smooth operators $h \in \mathrm{C}^\infty\left(\mathbb{R}^{2d}, \mathscr{B}(\mathscr{H}_0)\right)$ such that for all multi–indices α, β there exists $K_{\alpha,\beta} > 0$ s.t.

$$\left\| \partial_q^\alpha \partial_p^\beta h(p,q) \right\|_{\mathscr{B}(\mathscr{H}_0)} \leq K_{\alpha,\beta} \hbar^{-k} \left(1 + |p|^2 + |q|^2\right)^{\frac{m}{2}}. \tag{4.7}$$

This definition can be generalized by considering more general order function than $\left(1 + |p|^2 + |q|^2\right)^{\frac{m}{2}}$. We will henceforth use the shorthand S_m for the symbol class S^0_m.

Proposition 4.1 (Weyl quantization)**.** *The Bochner integral*

$$\left(\mathrm{Op}^{\mathrm{w}}_\hbar[h]\,\psi\right)(x) = \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^{2d}} h\left(\frac{x+y}{2}, \xi\right) \psi(y) \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x-y)\xi}\, \mathrm{d}y \mathrm{d}\xi, \tag{4.8}$$

where $\hbar \in (0, 1]$, *defines a continuous operator*

$$\mathrm{Op}^{\mathrm{w}}_\hbar[h] \;:\; \mathcal{S}\left(\mathbb{R}^d, \mathscr{H}_0\right) \to \mathcal{S}\left(\mathbb{R}^d, \mathscr{H}_0\right), \tag{4.9}$$

if $h \in \mathrm{S}_m\left(\mathbb{R}^{2d}, \mathscr{B}(\mathscr{H}_0)\right)$.

Proof. The following can be found in [DS99]. From the definition of the symbol classes, it is clear that the Bochner integral is well defined. The proof is a direct consequence of the definition of the symbol classes and the equality

$$\left(1 + |x-y|^2 + |\xi|^2\right)^{-1} \left(1 + \mathrm{i}\xi\,\hbar\partial_y - \mathrm{i}(x-y)\,\hbar\partial_\xi\right) \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x-y)\cdot\xi} = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x-y)\cdot\xi}, \tag{4.10}$$

which implies, after N successive steps that

$$\mathrm{Op}^{\mathrm{w}}_\hbar[h] = \int_{\mathbb{R}^{2d}} (1 + |x-y| + |\xi|)^{-N} (1 + |y|)^{-N} \mathscr{O}(1) \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x-y)\cdot\xi}\, \mathrm{d}\xi\, \mathrm{d}y, \tag{4.11}$$

since $h \in \mathrm{S}_m\left(\mathbb{R}^{2d}, \mathscr{B}(\mathscr{H}_0)\right)$. This implies in the norm of $\mathscr{B}(\mathscr{H}_0)$ the existence of positive $C_N < \infty$ s.t. $\forall N \in \mathbb{N}_0$

$$\left\| \mathrm{Op}^{\mathrm{w}}_\hbar[h]\,\psi \right\|_{\mathscr{B}(\mathscr{H}_0)} \leq C_N (1 + |x|)^{-N}. \tag{4.12}$$

A similar argument can be put forward for the derivatives proving continuity as a linear operator from $\mathcal{S}\left(\mathbb{R}^d, \mathscr{H}_0\right)$ to $\mathcal{S}\left(\mathbb{R}^d, \mathscr{H}_0\right)$.

□

We call a pseudo–differential operator elliptic with symbol h if the inverse of its symbol h^{-1} exists and

$$\exists C > 0,\, m > 0 \text{ s.t. } \|h(p,q)\|_{\mathscr{B}\left(\mathrm{L}^2\left(\mathbb{R}^d\right)\right)} \geq C\left(1+|p|^2+|q|^2\right)^{\frac{m}{2}}. \tag{4.13}$$

The following will also be useful.

Proposition 4.2. *Let h be a symbol in $\mathrm{S}_m\left(\mathbb{R}^{2d}, \mathscr{B}(\mathscr{H}_0)\right)$ such that $(h+\mathrm{i})$ is elliptic, then $\mathrm{Op}^{\mathrm{w}}_{\hbar}[h]$ is an essentially self-adjoint operator with domain $\mathcal{S}\left(\mathbb{R}^d, \mathscr{H}_0\right)$ if $\hbar$ is sufficiently small.*

This proposition is a slight adaption from [DS99], page 101, Proposition 8.5. It enables us to use the usual functional calculus of self–adjoint operators on $\mathrm{L}^2\left(\mathbb{R}^d\right)$. In particular, to smooth functions $f(p)$, $g(q)$ correspond operators $f\left(\widehat{p}\right)$ and $g(\widehat{x})$ in the conventional sense (f and g have Taylor series). Functions including products of the type qp are in this context dealt with in an acceptable way as their Weyl-quantization do not suffer from the problem of the canonical quantization, e.g., $\widehat{x}\widehat{p}$ and $\widehat{p}\widehat{x}$ differing from an additional factor $\mathrm{i}\hbar$. The above procedure produces a symmetric "ordering" of the operators, in this particular case $\frac{1}{2}\left(\widehat{x}\widehat{p}+\widehat{p}\widehat{x}\right)$.

An asymptotic expansion of a symbol $f \in \mathrm{S}^{k_0}_m$ is characterized by a sequence of symbols $f_i \in \mathrm{S}^{k_i}_m$ such that

$$f - \sum_{i=0}^{N-1} f_i \in \mathrm{S}^{k_N}_m \tag{4.14}$$

where k_i decreases monotonously such that $\lim_{i\to\infty} k_i = -\infty$. The corresponding equivalence relation will be denoted $\asymp$, i.e.,

$$f \asymp \sum_{i=0}^{\infty} f_i. \tag{4.15}$$

In many applications we will assume that a symbol f in the S^k_m has an asymptotic expansions in integer powers of $\hbar$

$$f \asymp \hbar^k \sum_{i\in\mathbb{N}_0} \hbar^i f_i. \tag{4.16}$$

as $\hbar \to 0$ in such a way that f_i are $\hbar$ independent. Such symbols will be called classical symbols and we will write $f \in S^{\mathrm{Cl},k}_m$. For an operator $\widehat{f} = \mathrm{Op}^{\mathrm{w}}_\hbar[f]$, where f has an asymptotic expansion of the type (4.16), f will denote the Weyl symbol of $\widehat{f}$. Moreover, $f_0 = \mathrm{symb}^{\mathrm{w}}_{\hbar,0}\left[\widehat{f}\right]$ will be called principal symbol and $f_1 = \mathrm{symb}^{\mathrm{w}}_{\hbar,1}\left[\widehat{f}\right]$ will be called the subprincipal symbol of $\mathrm{Op}^{\mathrm{w}}_\hbar[f]$.

We will need to define the so called Moyal product $\sharp_\hbar$ that is formally defined in the following way

$$\mathrm{Op}^{\mathrm{w}}_\hbar[f]\,\mathrm{Op}^{\mathrm{w}}_\hbar[g] \stackrel{\mathrm{def}}{=} \mathrm{Op}^{\mathrm{w}}_\hbar\left[f \sharp_\hbar g\right]. \tag{4.17}$$

The following characterization can be made.

Proposition 4.3 (Moyal product)**.** *The Moyal product*

$$f \sharp_\hbar g(\xi, x) = \mathrm{e}^{\frac{\mathrm{i}\hbar}{2}\left(\partial_\xi\partial_y - \partial_x\partial_\eta\right)} f(\xi, x) g(\eta, y)\Big|_{(\eta,y)=(\xi,x)} \tag{4.18}$$

is a map $\sharp_\hbar : S_m\left(\mathbb{R}^{2d}, \mathscr{H}_0\right) \times S_{m'}\left(\mathbb{R}^{2d}, \mathscr{H}_0\right) \to S_{m+m'}\left(\mathbb{R}^{2d}, \mathscr{H}_0\right)$ *that satisfies*

$$\mathrm{Op}^{\mathrm{w}}_\hbar\left[f \sharp_\hbar g\right] = \mathrm{Op}^{\mathrm{w}}_\hbar[f]\,\mathrm{Op}^{\mathrm{w}}_\hbar[g]. \tag{4.19}$$

We refer to the standard literature for a proof. See, e.g., [DS99]. This leads to a practical definition (Moyal commutator)

$$[f, g]_{\sharp,\hbar} \stackrel{\mathrm{def}}{=} f \sharp_\hbar g - g \sharp_\hbar f \tag{4.20}$$

with the nice property

$$\mathrm{Op}^{\mathrm{w}}_\hbar\left[[f, g]_{\sharp,\hbar}\right] = \left[\mathrm{Op}^{\mathrm{w}}_\hbar[f], \mathrm{Op}^{\mathrm{w}}_\hbar[g]\right]. \tag{4.21}$$

Furthermore, to each function in $L^2\left(\mathbb{R}^d\right)$, a complex valued function on $\mathbb{R}^d \times \mathbb{R}^d$ can be attributed through the Wigner transformation

$$W[\psi](p, q) = \int_{\mathbb{R}^d} \psi^*\left(q + \frac{y}{2}\right)\psi\left(q - \frac{y}{2}\right)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}py}\,\mathrm{d}y. \tag{4.22}$$

In particular, normalized Gaußian functions in $L^2\left(\mathbb{R}^d\right)$ are represented as normalized real $2d$ Gaußians, i.e., they are positive measures on $\mathbb{R}^d \times \mathbb{R}^d$.

classical		quantum
$\mathrm{T}^*\mathbb{R}^d$	$\longrightarrow$	$\mathrm{L}^2\left(\mathbb{R}^d\right)$
cotangent bundle		separable Hilbert space
$a \in \mathrm{S}_m\left(\mathbb{R}^{2d}, \mathscr{B}(\mathscr{H}_0)\right)$	$\longrightarrow$	$\mathrm{Op}^{\mathrm{w}}_\hbar[a]$
functions on phase space		self–adjoint operators
$[f, g]_{\sharp, \hbar}$	$\longrightarrow$	$\left[\mathrm{Op}^{\mathrm{w}}_\hbar[f], \mathrm{Op}^{\mathrm{w}}_\hbar[g]\right]$
Moyal commutator		commutator

Table 4.1: correspondence mediated by the Weyl quantization

The expectation value of an operator $\mathrm{Op}^{\mathrm{w}}_\hbar[f]$ with symbol f is hereby reduced to

$$\left\langle \psi, \mathrm{Op}^{\mathrm{w}}_\hbar[f]\,\psi \right\rangle = \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^{2d}} W[\psi](p,q) f(p,q)\,\mathrm{d}p\mathrm{d}q. \tag{4.23}$$

This equality can be used advantageously in certain calculations. The connection between symbols and their corresponding operators can be extended further. The integral kernel $K_{\widehat{f}}$ of $\mathrm{Op}^{\mathrm{w}}_\hbar[f]$ can be expressed as

$$K_{\widehat{f}}(x,y) = \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} f\left(p, \frac{x+y}{2}\right) \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(x-y)}\,\mathrm{d}p. \tag{4.24}$$

The symbol of an operator $\widehat{f}$ is given by

$$\mathrm{symb}^{\mathrm{w}}_\hbar\left[\widehat{f}\right](p,q) = \int_{\mathbb{R}^d} K_{\widehat{f}}\left(q + \frac{z}{2}, q - \frac{z}{2}\right) \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}pz}\,\mathrm{d}z. \tag{4.25}$$

4.2 The "classical" in semiclassical

Assuming that an observable $a \in \mathrm{S}^{\mathrm{Cl},0}_m$ and a Hamilton function $h \in \mathrm{S}^{\mathrm{Cl},0}_n$ have asymptotic expansions of the type (4.16), the Moyal commutator can be calculated to leading order in $\hbar$ to

$$[h, a]_{\sharp, \hbar}(\xi, x) \asymp \mathrm{i}\hbar\{h_0, a_0\}_{(\xi,x)} + \mathscr{O}\left(\hbar^2\right). \tag{4.26}$$

In view of the Heisenberg equation of motion in quantum mechanics and Hamilton's equation of motion in classical mechanics, this suggests that classical dynamics and quantum mechanics are close to each other as $\hbar \to 0$. Such statements are covered by what is commonly called the *Bohr correspondence principle*. We will illustrate this in the following way.

We consider here scalar classical symbols a and h in $S^{Cl,0}_m$. We will denote by $\mathscr{U}$ the unitary evolution generated by $\mathrm{Op}^{\mathrm{w}}_{\hbar}[h]$. We simply calculate

$$\begin{aligned}\widehat{R}(t) &= \mathscr{U}^*(t)\mathrm{Op}^{\mathrm{w}}_{\hbar}[a]\,\mathscr{U}(t) - \mathrm{Op}^{\mathrm{w}}_{\hbar}\left[a\circ\Phi^t_{h_0}\right] &(4.27)\\ &= \int_0^t \frac{\mathrm{d}}{\mathrm{d}s}\Big(\mathscr{U}^*(s)\mathrm{Op}^{\mathrm{w}}_{\hbar}\left[a\circ\Phi^{t-s}_{h_0}\right]\mathscr{U}(s)\Big)\,\mathrm{d}s, &(4.28)\end{aligned}$$

i.e., the discrepancy when interchanging evolution and quantization. Differentiating in the integrand, we find

$$\widehat{R} = \int_0^t \mathscr{U}^*(s) r(t,s)\mathscr{U}(s)\,\mathrm{d}s, \tag{4.29}$$

with

$$r(t,s) = \frac{\mathrm{i}}{\hbar}\left[\mathrm{Op}^{\mathrm{w}}_{\hbar}[h], \mathrm{Op}^{\mathrm{w}}_{\hbar}\left[a\circ\Phi^{t-s}_{h_0}\right]\right] - \mathrm{Op}^{\mathrm{w}}_{\hbar}\left[\frac{\mathrm{d}\left(a\circ\Phi^{t-s}_{h_0}\right)}{\mathrm{d}s}\right] \tag{4.30}$$

where these last statement comes from the fact $\mathrm{Op}^{\mathrm{w}}_{\hbar}[h]$ generates $\mathscr{U}$. Using the properties of the Moyal commutator and the fact that the classical flow $\Phi^t_{h_0}$ is generated by h_0, we may write this

$$\widehat{R}(t) = \int_0^t \mathscr{U}^*(s)\mathrm{Op}^{\mathrm{w}}_{\hbar}\left[\frac{\mathrm{i}}{\hbar}\left[h, a\circ\Phi^{t-s}_{h_0}\right]_{\sharp,\hbar} - \{h_0, \Phi^{t-s}_{h_0}\}\right]\mathscr{U}(s)\,\mathrm{d}s.$$

The integrand is of order $\mathscr{O}(\hbar)$. Now, taking the $\mathrm{L}^2\left(\mathbb{R}^d\right)$ norm we find

$$\left\|\mathscr{U}^*(t)\mathrm{Op}^{\mathrm{w}}_{\hbar}[a]\,\mathscr{U}(t) - \mathrm{Op}^{\mathrm{w}}_{\hbar}\left[a\circ\Phi^t_{h_0}\right]\right\|_{\mathrm{L}^2\left(\mathbb{R}^2\right)} \leq C_t\,\hbar, \tag{4.31}$$

where it can be shown that C_t is bounded for finite times(see e.g. [BR02]). Such results are usually called semiclassical Egorov theorems in analogy to a contribution of the latter [Ego69]. We have shown modulo errors $\mathscr{O}(\hbar)$ that the evolution and quantization commute when considering the expectation values of operators. In particular the expectation values of the quantum evolutions coincide with the values of the evolved classical observables in the limit $\hbar \to 0$. Such results can be shown modulo errors $\mathscr{O}(\hbar^\infty)$ considering the evolution of each subsymbol of an operator (see e.g. [BR02] and references therein). Such results are also available for matrix valued symbols [PST03, BG04].

4.3 Construction of approximate evolution

Quadratic forms play a particular role in quantum mechanics. The evolution generated by quadratic Hamiltonians can be constructed exactly using Gaußian states. Furthermore, as we shall see these evolutions have astounding properties. The ultimate aim of this section is to introduce the propagation of coherent states. This scheme has emerged from ideas of Heller[Hel75] and Hepp [Hep74] and have been pursued in more stringent footing by Hagedorn [Hag81, Hag85], Combescure and Robert [CR97] amongst others.

For this purpose, we introduce the following family of Gaußians, commonly called squeezed states.

4.3.1 Gaußian wave packets

We consider wave packets of the form

$$\psi_Z^{(p,q)}(x) := \frac{\det(\mathrm{Im}(Z))^{\frac{1}{4}}}{(\pi\hbar)^{\frac{d}{4}}} e^{\frac{i}{\hbar}\left(p^T(x-q)+(x-q)^T\frac{Z}{2}(x-q)\right)}, \tag{4.32}$$

where $Z \in \Sigma_d$, $\begin{pmatrix} p \\ q \end{pmatrix} \in \mathbb{R}^{2d}$. By Σ_d, we mean the $d-$dimensional Siegel upper half space, i.e., the set of symmetric $d \times d$ matrices with positive, non-degenerate imaginary part [Fol89]. The matrix Z describes the shape of the wave packet and it should be underlined that it is independent of $\hbar$. The Wigner transform of $\psi_Z^{(p,q)}$ is a $2d$ Gaußian centered around $X = \begin{pmatrix} p \\ q \end{pmatrix}$, given by

$$W\left[\psi_Z^X\right](Y) = \left(\frac{1}{\pi\hbar}\right)^d \exp\left(-\frac{1}{\hbar}(Y-X)^T G(Y-X)\right),$$

where

$$G := \begin{pmatrix} \mathrm{Im}(Z)^{-1} & -\mathrm{Im}(Z)^{-1}\mathrm{Re}(Z) \\ -\mathrm{Re}(Z)\mathrm{Im}(Z)^{-1} & \mathrm{Im}(Z)+\mathrm{Re}(Z)\mathrm{Im}(Z)^{-1}\mathrm{Re}(Z) \end{pmatrix} \tag{4.33}$$

is also independent of $\hbar$.

The advantage of Gaußian states will become apparent in the next section.

4.3.2 A quadratic approximation scheme

We consider some quantized Hamiltonian, defined as above, i.e., as the Weyl quantization of a smooth function $h \in \mathrm{S}_m$. The idea here is to approximate this

Hamiltonian with a simpler, quadratic one making use of the above Gaußians. The goal being to use known facts about quadratic Hamiltonians to approximate the evolution, namely:

1. The evolution of a the Gaußian generated by a quadratic Hamiltonian remains a Gaußian,
2. the evolution can be computed explicitly.

The finesse is to allow the approximating quadratic Hamiltonian to be time dependent.

We assume that h generates a flow Φ_h^t with trajectory $X_t = \Phi_h^t(X_0)$, and define the time dependent quadratic Hamiltonian

$$H_2(t, Y) := h(X_t) + (Y - X_t)^T h'(X_t) + \frac{1}{2}(Y - X_t)^T h''(X_t)(Y - X_t), \tag{4.34}$$

i.e., the second order expansion of h around the trajectory X_t, where h' is the gradient and h'' is the Hessian of $h(X)$.

The quantization of H_2 generates a unitary group $\mathcal{U}_2(t)$. Its action on a Gaußian can be summarized in the following way [Fol89],

$$\mathcal{U}_2(t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Theta(t)} \widehat{\mathcal{T}}(X_t) \widehat{\mathcal{M}}(S_t), \tag{4.35}$$

where

$$\widehat{\mathcal{T}}(X_t) = \exp\left(\frac{\mathrm{i}}{\hbar}(p_t \widehat{x} - \widehat{p} q_t)\right) \tag{4.36}$$

is the translation operator as described above. We have here written the trajectory in canonical coordinates (p_t, q_t). The metaplectic operator (see appendix B) $\widehat{\mathcal{M}}(F)$ is the quantization of a linear symplectomorphism on $\mathbb{R}^{2d}$ given by the symplectic matrix F. These operators form a double-valued unitary representation of the linear symplectomorphism of $\mathbb{R}^{2d}$. S_t denotes the flow differential. The classical flow Φ_h^t is a symplectomorphism which ensures that the flow differential is a symplectic matrix. Θ is given by the action of the full Hamiltonian and the corresponding Maslov index μ (see section 4.7), i.e.,

$$\Theta(t) = \mathcal{S}(t) - \hbar \frac{\pi \mu}{4}. \tag{4.37}$$

An explicit calculation gives the new Gaußian

$$\mathcal{U}_2(t) \psi_{Z_0}^{X_0}(x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Theta(t)} \psi_{Z_t}^{X_t}(x), \tag{4.38}$$

now centered around X_t and with quadratic from

$$Z_t = (A_t Z_0 + B_t)(C_t Z_0 + D_t)^{-1}, \tag{4.39}$$

with the flow differential

$$S_t = \begin{pmatrix} A_t & B_t \\ C_t & D_t \end{pmatrix} \in \mathrm{Sp}(2d, \mathbb{R}). \tag{4.40}$$

Furthermore, it can be verified that the Wigner function of the Gaußian will have a quadratic form described by the matrix

$$G_t = \left(S_t^{-1}\right)^T G_0 S_t \tag{4.41}$$

at time t.

Remark 4.1. *If S_t is orthogonal, the approximate Gaußian profile will be the initial one. It will just be rotated and translated in phase space.*

4.3.3 Semiclassical errors

Having described the approximate state, the task of estimating the errors that this approximation generates remains. Such results have been produced by Hagedorn [Hag81, Hag85, HJ99, HJ00], as well as Combescure and Robert [CR97] to name a few.

To state the result of this section, we need the following states:

$$\Psi^{(N)}(t, x) := \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Theta(t)} \sum_{0 \le j \le N} \hbar^{\frac{j}{2}} \pi_j\left(X_t, \frac{x}{\sqrt{\hbar}}, t\right) \psi_{Z_t}^{X_t}(x), \tag{4.42}$$

where $\pi_j\left(X_t, \frac{x}{\sqrt{\hbar}}, t\right)$ are polynomials in $x/\sqrt{\hbar}$ and X_t of degree smaller than or equal to $3j$ with time dependent coefficients.

Theorem 4.1 (Combescure, Robert)**.** *Assuming the Hamiltonian function $h \in \mathrm{S}_m$ and an initial Gaußian state $\psi_{Z_0}^{X_0}$ centered in the phase space representation at $X_0 \in \mathrm{T}^*\mathbb{R}^d$, then for every $N \in \mathbb{N}$ there exists $C < \infty$ such that $\forall\, \hbar \in (0, \hbar_0]$, $\hbar_0 > 0$,*

$$\left\| \mathcal{U}(t)\psi_{Z_0}^{X_0} - \Psi^{(N)}(t) \right\| \le C_N \hbar^{\frac{N+1}{2}} t \mathrm{e}^{3\gamma t}, \tag{4.43}$$

where γ is the Lyapunov exponent of the classical motion and $\mathrm{Op}_\hbar^{\mathrm{w}}[h]$ generates $\mathcal{U}(t)$.

We refer to [CR97] for the proof.

The use of the Lyapunov exponents (see sec 2.5) comes from the stability of the classical orbits, or in other words, a bound for the Hilbert-Schmidt norm of the flow differential.

4.4 Localization

We wish to characterize the times for which the above approximation holds. As we mentioned earlier we will not merely demand that the errors of (4.43) remain small but also stress that the state be localized, meaning, it makes no sense approximating a non localized particle with a point particle (see [Str08]).

Of particular interest to us is the width of the propagated initial Gaußian, i.e., we are particularly interested in the operator

$$\widehat{s} := \mathrm{Op}^{\mathrm{w}}_{\hbar}\left[p^2 + q^2\right]. \tag{4.44}$$

Integrating the approximate Gaußian, $\psi^{Z_t}_{X_t}(x)$, one finds that the semiclassical width is

$$\sigma_t(X_0;\,\hbar) := \Delta x^2(\hbar,\,t) + \Delta p^2(\hbar,\,t) = \frac{\hbar}{2}\mathrm{tr}\big(G_t\big), \tag{4.45}$$

where we have used the approximate variance

$$\Delta x^2 = \left\langle \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Theta(t)}\psi^{X_t}_{Z_t},\, \widehat{x}^2\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Theta(t)}\psi^{X_t}_{Z_t}\right\rangle - \left\langle \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Theta(t)}\psi^{X_t}_{Z_t},\, \widehat{x}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Theta(t)}\psi^{X_t}_{Z_t}\right\rangle^2, \tag{4.46}$$

and similarly for the momentum operator. The width can explicitly be written with the help of the flow differential. Using (4.41) we get

$$\sigma_t \;\leq\; \sigma_0 \|S_t\|^2_{\mathrm{HS}}.$$

One has, as for the error (4.43), to rely on properties of the flow differential. From the definition of a Lyapunov exponent, one can directly state that if $\gamma \neq 0$, the width will grow exponentially in time.

4.4.1 Revivals

We here further assume that the Hessian $h''\big(X_t\big)$ is $T-$periodic, i.e.,

$$h''\big(X_t\big) = h''\big(X_{t+T}\big), \quad \forall t \in \mathbb{R}. \tag{4.47}$$

An example is unbounded classical motion in a one dimensional periodic potential V. Although the flow itself is not periodic, the Hessian

$$h''\big(X_t\big) = V''\big(q_t\big) \tag{4.48}$$

will be periodic. This implies amongst others that the classical period, which we define by the period of the Hessian, does not coincide in general with a period of the Hamiltonian flow. In the event of periodic bounded motion, the period of both the Hessian and the flow will, however, coincide.

The periodicity condition (4.47) will allow us to make use of Floquet theory since the flow differential of the classical motion will satisfy the ODE

$$\begin{aligned} \frac{\mathrm{d}S_t}{\mathrm{d}t} &= \mathcal{J}h''(X_t)S_t, \\ S_0 &= \mathbb{1}_{2d\times 2d}, \end{aligned}$$

with periodic coefficients, and hence it has a Floquet solution of the kind

$$\begin{aligned} S_t &= M^{-1}\mathrm{e}^{\Lambda t}MP_t, \quad M\in \mathrm{GL}(2d,\mathbb{C}), \\ P_t &= P_{t+T}. \end{aligned}$$

The initial conditions dictate that $P_0 = \mathbb{1}_{2d\times 2d}$. In sections 4.4.1 and 4.4.2 we consider the case where the Floquet matrix Λ is diagonalizable. In section 4.4.3 we discuss the case when the Floquet matrix is not diagonalizable.

As the heading indicates, we wish to describe some recurrences.

Definition 4.2 (Classical revival)**.** A classical revival at a time $t \neq 0$ is the event that the approximate Gaußian given above is the initial one up to a phase factor, i.e.,

$$\psi^{X_t}_{Z_t} = \mathrm{e}^{\mathrm{i}\alpha_t}\psi^{X_0}_{Z_0},\ \alpha_t\in\mathbb{R}.$$

We first make a statement about the width of the approximate state.

Proposition 4.4. *If $h''(X_t)$ is periodic with smallest period T and the Floquet matrix corresponding to S_t is diagonalizable with purely complex exponents then the width of a Gaußian propagated semiclassically by $\mathcal{U}_2(t)$ will remain unchanged at multiples of T.*

Proof. We assume here that Λ has eigenvalues $\mathrm{e}^{2\pi\lambda_i\frac{t}{T}}$, $\lambda_i\in\mathbb{C}$. By the property of Floquet solutions one concludes directly that

$$S_{kT} = M^{-1}\mathrm{e}^{kT\Lambda}M, \quad \forall k\in\mathbb{Z},$$

for multiples k of the minimal period T.

Furthermore, the real fundamental matrix defined by $S_t \in \mathrm{Sp}(2d,\mathbb{R})$ has a unique polar decomposition, i.e., there exists [Fol89] an orthogonal matrix $\mathcal{Q}_t\in\mathrm{O}(2d)\cap\mathrm{Sp}(2d,\mathbb{R})$ and a positive definite matrix $\mathcal{P}_t\in\mathrm{Sp}(2d,\mathbb{R})$ such that

$$S_t = \mathcal{Q}_t\mathcal{P}_t.$$

The width of the approximate squeezed state at time t is (see eq. (4.45) and and (4.41))

$$\sigma_t(\hbar) = \mathrm{tr}\Big(\big(S_t^{-1}\big)^T G_0 S_t^{-1}\Big),$$

and since any symplectic matrix A satisfies (see appendix A or [Fol89])

$$A^{-1} = \mathscr{J} A^T \mathscr{J}^{-1},$$

and $\mathcal{Q}_t \in \mathrm{O}(2d)$, we have,

$$\sigma_t(\hbar) = \frac{\hbar}{2}\mathrm{tr}\Big(\mathcal{Q}_t \mathcal{P}_t \mathcal{J}^T G_0 \mathcal{J} \mathcal{P}_t^T \mathcal{Q}_t^T\Big) = \frac{\hbar}{2}\mathrm{tr}\Big(\mathcal{P}_t \mathscr{J}^T G_0 \mathscr{J} \mathcal{P}_t^T\Big). \tag{4.49}$$

We are hence confronted with two cases:

- S_{kT} is orthogonal, i.e., $\mathcal{P}_{kT} = \mathbb{1}_{2d\times 2d}$. This corresponds to

$$\sigma_{kT}(\hbar) = \frac{\hbar}{2}\mathrm{tr}(G_0) = \sigma_0(\hbar), \quad \forall k \in \mathbb{Z}. \tag{4.50}$$

  The orthogonality of S_{kT} implies that it has $2d$ singular values 1. It is furthermore similar to $\mathrm{e}^{kT\Lambda}$ $\big(F_{kT} = \mathbb{1}_{2d\times 2d}\big)$, which hence is unitary so the Floquet exponents $\frac{2\pi\lambda_i}{T}$ are either purely complex or zero. One notes that

$$\begin{aligned} S_t^* S_t &= P_t^* \big(M^{-1}\mathrm{e}^{t\Lambda}M\big)^* M^{-1}\mathrm{e}^{t\Lambda}M P_t & (4.51)\\ &= P_t^* P_t, & (4.52)\end{aligned}$$

  by unitarity of $\mathrm{e}^{\Lambda t}$. Thus $||S_t||_{\mathrm{HS}}$ is uniformly bounded and the Lyapunov exponent of the classical trajectories is zero. The classical motion is linearly stable.

- $\mathcal{P}_{kT} \neq \mathbb{1}_{2d\times 2d}$, which corresponds to

$$\begin{aligned}\sigma_{kT}(\hbar) &= \frac{\hbar}{2}\mathrm{tr}\Big(\mathcal{P}_{kT}\mathscr{J}^T G_0 \mathcal{J}\mathcal{P}_{kT}^T\Big)\\ &> \sigma_0(\hbar),\end{aligned}$$

  since $\mathcal{P}_t \in \mathrm{Sp}(2d, \mathbb{R})$ is strictly positive definite. Since P is periodic, one concludes that $\mathrm{e}^{\Lambda t}$ is not unitary. At least one singular value of Λ will hence have a non-vanishing real part. The Lyapunov exponent of the trajectory will hence be non-vanishing.

□

The periodicity of P_t enables us to make the following observation.

Corollary 4.1 (semiclassical recurrences)**.** *If $h''(X_t)$ is periodic, the Floquet matrix Λ corresponding to (3.6) is diagonalizable and has purely imaginary eigenvalues, $\mathcal{U}_2(t)\psi_{X_0}^{Z_0}$ will have classical revivals at classical periods. In particular, if the corresponding classical flow is periodic, classical revivals will occur at each period.*

Proof . We make the distinction between two cases, the last being the general one:

1. If the (purely complex) Floquet exponents are rationally dependent, there exist some multiples
$$T_R = n_R T, \quad n_R \in \mathbb{Z},$$
of the classical period T such that the orthogonal transformation reduces to unity. Indeed, if n_R is the smallest common multiple of the denominators of the sequence $\{\lambda_i\}$ defined by the Floquet exponents, i.e.,
$$\lambda_i n_R \in \mathbb{N}_0, \forall i,$$
we find
$$\begin{aligned} M^{-1}\mathrm{e}^{\Lambda T_R}M &= M^{-1}\mathrm{diag}\left\{\mathrm{e}^{2\pi i n_i}\right\}M, \quad n_i \in \mathbb{Z}, && (4.53)\\ &= \mathbb{1}_{2d\times 2d}. && (4.54)\end{aligned}$$
The semiclassical approximation of the evolution is then the initial Gaußian, if it is localized at the initial point X_0. This is the case if the flow is periodic. In this case we have a classical revival.

2. In the general case, i.e., if the Floquet exponents are not linearly dependent, we have to use some ergodic theory. Recall that the matrix Z_t is given by a linear fractional transformation, i.e.,
$$Z_{kT} = \left(A_{kT}Z_0 + B_{kT}\right)\left(C_{kT}Z_0 + D_{kT}\right)^{-1}.$$
By assumption, the eigenvalues of Λ are purely imaginary, hence $S_{kT} \sim \mathrm{e}^{\Lambda kT}$ is unitary. Assuming the eigenvalues to be $\mathrm{e}^{\mathrm{i}\ell_i\frac{2\pi}{T}} = \mathrm{e}^{\lambda_i\frac{2\pi}{T}}$ with $\ell_i \in \mathbb{R}$, the linear factional transformation giving the matrix Z at time kT can be seen in terms of the map
$$\begin{aligned} \mathsf{e} \;:\; & \mathbb{T}^d \to \Sigma_d \\ & \ell kT \mapsto Z_{kT}. \end{aligned}$$

The endomorphism

$$\begin{aligned}\tau \;:\; & \mathbb{T}^d \to \mathbb{T}^d \\ & L \mapsto L + \ell,\end{aligned}$$

where $(L_i + \ell_i)$ is defined modulo 1, is known to be ergodic with respect to Lebesgue measure on the $d-$torus since the frequencies ℓ_i are rationally independent [Pol93]. In this notation we have $Z_0 = \mathsf{e}(0) = \mathsf{e}(L(0))$. It follows that for every $\varepsilon > 0$ there exist some $n \in \mathbb{Z}$ such that $||\mathsf{e} \circ \tau^n(0) - \mathsf{e}(0)|| < \varepsilon$, implying

$$\forall \varepsilon > 0, \exists n \in \mathbb{Z}: \quad ||Z_{nT} - Z_0|| < \varepsilon,$$

i.e., Z_{kT} is quasi–periodic. One concludes that the initial shape of the state will, up to some small error, reoccur at some multiple of the classical period, if the Floquet exponents of the flow differential are purely imaginary.

□

As long as the errors of the approximation of section 4.3.3 remain small and the state is localized, approximate revivals will occur also for the exactly propagated states. Note that the conditions for these revivals only describe classical quantities, i.e., all quantities are $\hbar-$independent.

The main ingredient here is that the Floquet exponents are purely imaginary. In particular, if S_t is periodic we have revivals at each classical period if the flow is periodic. This does not, however, exclude the event of revivals if the motion is unbounded since the flow differential can also then be second periodic.

For bounded motion, corresponding to a quantum Hamiltonian with discrete spectrum, the event of revivals can be shown with rather general arguments [Ono49, BL57] and can be seen as a result of

$$||(1 - \mathcal{U}(t))\psi_0|| = \left\| \sum_{i \in \mathbb{N}_0} c_i \left(1 - \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} E_i t}\right) \varphi_i \right\|, \quad (c_0, c_1, c_2, ...) \in \ell^2(\mathbb{N}_0), \quad (4.55)$$

being an almost periodic function [Boh24, Boh25]. Such results are often called "quantum recurrences". This refers to its classical counterpart, the Poincaré recurrence theorem (see, e.g. [Arn78]).

More recently Averbuck and Perelman [AP89] discussed the behavior of wave packets in the classical limit. One expects that the spectrum of the Hamiltonian of a bounded particle will be locally well described by that of a harmonic oscillator. Their discussion started by considering a slightly perturbed

equidistant spectrum. This consideration produces revivals on two scales. On the scale of the classical mechanics, induced through the underlying equidistant spectrum, revivals occur at the periods of the classical flow, i.e., what we have described as classical revivals. The second kind of revivals can occur on larger time scales. In particular, they occur beyond the so–called Ehrenfest time which is not covered by our arguments (see [CR07] and below).

4.4.2 A uniform bound for the flow differential

As we mentioned in the last section, we also need localization of the approximate state to be able to make statements about the exact one. We restrain to the case where Floquet exponents are purely imaginary.

Lemma 4.1. *If $H''(X_t)$ is $T-$periodic and the Floquet exponents of S_t are purely imaginary then the width $\sigma_t(\hbar)$ of a Gaußian state propagated by $\mathcal{U}_2(t)$ satisfies the following uniform bound*

$$\sigma_t(\hbar) \leq \mathrm{e}^{\varkappa}\sigma_0(\hbar), \forall t \in \mathbb{R}, \tag{4.56}$$

where $\varkappa$ is defined by

$$\varkappa := 2T \sup_{t\in[0,T]} \left\| \mathscr{J} H''(X_t) \right\|_{\mathrm{HS}}.$$

Proof. We consider (3.6) starting at some initial time kT, $k \in \mathbb{Z}$. S_{t+kT} satisfies the Grönwall inequality

$$\left\| S_{t+kT} \right\|_{\mathrm{HS}} \leq \|S_{kT}\|_{\mathrm{HS}} \mathrm{e}^{\varkappa}, \forall t \in [0, T],$$

during a classical period T where

$$\varkappa = 2T \sup_{t\in[0,T]} \left\| \mathscr{J} H''(X_t) \right\|_{\mathrm{HS}}.$$

Furthermore,

$$\begin{aligned} \sigma_t(\hbar) &= \frac{\hbar}{2}\mathrm{tr}\left(S_t \mathscr{J}^T G_0 \mathscr{J} S_t^T\right) \\ &= \frac{\hbar}{2}\mathrm{tr}\left(G_0 S_t^T S_t\right) \leq \frac{\hbar}{2}|\mathrm{tr}(G_0)|\,\|S_t\|_{\mathrm{HS}}^2. \end{aligned}$$

Hence

$$\sigma_t(\hbar) \leq \frac{\hbar}{2}|\mathrm{tr}(G_0)|\,\mathrm{e}^{\varkappa}, \tag{4.57}$$

if S_t has purely imaginary Floquet exponents since in this case $\sigma_0(\hbar) = \sigma_{kT}(\hbar)$, according to Proposition 4.4.

We conclude with this choice that

$$\sigma_t(\hbar) \leq K\sigma_0(\hbar), \tag{4.58}$$

uniformly in time.

□

If S_t is not orthogonal at the classical periods T, the latter bound takes the form

$$\sigma_t(\hbar) \quad \leq \quad K\sigma_0(\hbar)\mathrm{e}^{\frac{4\pi}{T}\max_i\left(\mathrm{Re}\left(\lambda_i\right)\right)|t|}$$

where $\frac{2\pi}{T}\lambda_i$ are the corresponding Floquet exponents of S_t which is nothing else than a Lyapunov inequality where $\max_i\left(\mathrm{Re}\left(l_i\right)\right)$ plays the role of the Lyapunov exponent. Using the fact that what we are approximating is the Hilbert-Schmidt norm of the flow differential one can furthermore state the existence of a constant $C > 0$ such that

$$\frac{\mathrm{e}^{\frac{4\pi}{T}\max_i\left(\mathrm{Re}\left(\lambda_i\right)\right)|t|}}{C} \quad \leq \sigma_t(\hbar) \leq \quad C\mathrm{e}^{\frac{4\pi}{T}\max_i\left(\mathrm{Re}\left(\lambda_i\right)|t|\right)},$$

which determines the asymptotic behavior of the width in that case.

We remark that the lower bound in (4.56) is attained if the classical period is null, i.e., if the Hamiltonian has a constant Hessian $H''\left(X_t\right)$. This is satisfied by the harmonic oscillator. Then the flow differential S_t is an orthogonal matrix for all times. It is well known that the propagation is dispersion-less in this case.

4.4.3 The case of a non-diagonalizable Floquet matrix

Up to now, we have only studied the case where the solutions of (3.6),

$$S_t = M^{-1}\mathrm{e}^{\Lambda t}MF_t,$$

were represented by a diagonalizable Floquet matrix Λ. In general, this is not the case. Λ can, however, be put in Jordan normal form with block multipliers $\mathrm{e}^{\lambda_i t}$. The latter coincide with our definition of Floquet exponents if Λ is diagonalizable. We call λ_i Floquet exponents also in that case. If Λ is not diagonalizable, it is well known that the entries of S_t are a product of the block multipliers and polynomials in t with periodic coefficients. The degree of these polynomials will be determined by dimensions of the blocks of the Floquet matrix (see, e.g., [CL55]). We briefly discuss the non-diagonalizable case now.

If the Floquet exponents have non-vanishing real parts, it is clear that the behavior will be that of a chaotic classical motion since, at least asymptotically, the flow differential has exponential behavior.

If the real parts of the Floquet exponents vanish, the behavior of S_t will not be second periodic as in the diagonalizable case because of the additional polynomial element. However, one obtains a polynomial bound for S_t, which implies regular classical motion. One will also not have the classical revivals for the approximate state that we described earlier for the diagonalizable case since, clearly, $S_{kT} \notin \mathrm{O}(2d)$.

4.5 The Ehrenfest time

We discuss here the results of the last three sections in view of the errors of the approximation in 4.3.3, i.e., we wish to discuss properties of the approximate state $\mathscr{U}_2(t)\psi_{X_0}^{Z_0}$ in relation to the exactly evolved state $\mathscr{U}(t)\psi_{X_0}^{Z_0}$. In particular, we will see that the stability of the classical dynamics induce different time scales for the validity of the approximation.

With the propagation theorem of Combescure and Robert, the errors

$$\Delta(t) := \left\langle \mathscr{U}(t)\psi_{X_0}^{Z_0}, \widehat{s}\left(\mathscr{U}(t)\psi_{X_0}^{Z_0}\right)\right\rangle - \left\langle \mathscr{U}_2(t)\psi_{X_0}^{Z_0}, \widehat{s}\left(\mathscr{U}_2(t)\psi_{X_0}^{Z_0}\right)\right\rangle \tag{4.59}$$

for propagating observables $\widehat{s}$ can be approximated explicitly. We wish to characterize the times for which the errors (4.59) are of order $\hbar^\alpha$, with $\alpha > 0$, while making sure that the exact state remains localized.

We first treat unstable classical motion, where the Lyapunov exponent, or here the real part of the Floquet exponents, is not vanishing and we have a bound of the type

$$||S_t||_{\mathrm{HS}} \leq C\mathrm{e}^{\gamma|t|}. \tag{4.60}$$

This means that σ_t grows like $\mathrm{e}^{2\gamma t}$, whereas the errors are bounded by $Ct\mathrm{e}^{3\gamma t}$. In view of (4.43),

$$\left\| \mathscr{U}(t)\psi_{Z_0}^{X_0} - \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Theta(t)}\psi_{Z_t}^{X_t} \right\| \;\leq\; C\hbar^{\frac{1}{2}}t\mathrm{e}^{3\gamma t}, \tag{4.61}$$

the errors will be of order $\mathscr{O}(\hbar^\alpha)$ for times $T_E(\hbar) \propto |\ln(\hbar)|$ as $\hbar \to 0$. $T_E(\hbar)$ is usually called the Ehrenfest time, or quantum break time. Clearly, one can successfully approximate quantum dynamics by classical dynamics up to such times.

One can also define the Ehrenfest time for a much more restrained type of classical behavior, namely, regular motion. As we have seen we have to differentiate between two types of behaviors. If the flow differential has a Floquet

matrix that is diagonalizable, we have a constant bound for the flow differential. If the Floquet matrix is not diagonalizable, or the motion is regular but $h''(X_t)$ is not periodic, we may only attribute a polynomial bound to the flow differential.

If we have a constant bound for the flow differential, it is clear that the state will remain localized up to the generated errors if the bound between classical periods is small enough. By Lemma 4.1 this is satisfied if

$$\varkappa = 2T \sup_{t\in[0,T]} \left\| \mathcal{J} H''(X_t) \right\|_{\mathrm{HS}} \tag{4.62}$$

is sufficiently small. We characterize the times up to which a constant error is attained. Considering (4.61) in this case with an error χ

$$\chi \propto \hbar^{\frac{1}{2}} t, \tag{4.63}$$

we see that the Ehrenfest time will be of the order $T_E(\hbar) \propto \hbar^{-\frac{1}{2}}$ as $\hbar \to 0$.

If we have a polynomial bound of the form $\mathcal{O}(t^\alpha)$ for the flow differential, the errors will be bounded by

$$\left\| \mathcal{U}(t)\psi_{Z_0}^{X_0} - \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\Theta(t)}\psi_{Z_t}^{X_t} \right\| \;\leq\; C_{Err}\hbar^{\frac{1}{2}} t^{3\alpha+1}, \quad \text{as} \quad \hbar \to 0. \tag{4.64}$$

For an error χ we have

$$\chi \propto \hbar^{\frac{1}{2}} t^{3\alpha+1}. \tag{4.65}$$

The width will grow like

$$\sigma_t \propto \hbar t^{2\alpha}, \quad \text{as} \quad \hbar \to 0. \tag{4.66}$$

The Ehrenfest time will be given asymptotically by the smaller times generated by the two bounds, i.e., we find

$$T_E \propto \hbar^{-\lambda} \tag{4.67}$$

where

$$\lambda = \max\left(\frac{1}{2(3\alpha+1)}, \frac{1}{2\alpha}\right). \tag{4.68}$$

Thus, if $\alpha < \frac{1}{2}$, $\lambda = \frac{1}{2(3\alpha+1)}$ else we have $\lambda = \frac{1}{2\alpha}$.

We summarize the results in the following way.

Theorem 4.2 (Ehrenfest time). *Assume* $\mathrm{Op}^{\mathrm{w}}_{\hbar}[h]$ *with* $h \in \mathrm{S}_m$ *generates the unitary group* $\mathcal{U}(t)$. *Then, the approximation of* $\mathcal{U}(t)$ *by* $\mathcal{U}_2(t)$ *given by the construction of section 4.3.2 will be valid up to the Ehrenfest time*

$$T_E(\hbar) \propto |\ln(\hbar)| \tag{4.69}$$

asymptotically as $\hbar \to 0$. *The width of the state grows like* $\mathrm{e}^{2\gamma t}$ *up to* T_E *where* $\gamma > 0$ *is the Lyapunov exponent of the corresponding classical trajectory.*

If the classical dynamics is not chaotic, i.e., $\gamma = 0$ *and* $\varkappa$ *given by (4.56) is small enough, we have* $T_E \propto \hbar^{-\lambda}$ *where*

$$\lambda = \max\left(\frac{1}{2(3\alpha+1)}, \frac{1}{2\alpha}\right) \tag{4.70}$$

and α *is the degree of the asymptotic polynomial bound of the flow differential. The width of the exact state will behave like* $\hbar t^{2\alpha}$ *up to* $T_E(\hbar)$ *in this particular case.*

We have here just stated the result of the above discussion. The case of bounded flow differential, i.e., $\alpha = 0$ is now a special case of a polynomial bound. Now that we have all aspects of the approximation under control, we may state the following for the exact state.

Theorem 4.3 (Classical revivals). *Let* h *be a classical Hamiltonian such that*

$$h''(X_{t+T}) = h''(X_t), \tag{4.71}$$

where T *is minimal with this property. Then the exactly propagated state will experience classical revivals with small errors at some multiples of* T *up to the Ehrenfest time. The width of the exactly propagated state will, up to small errors, be the same at some multiples of* T. *In particular, if the flow differential is periodic, such classical revivals will occur at each classical period.*

This theorem is a consequence of Theorem 4.2, Lemma 4.1 and Corollary 4.1. We wish to stress that we have defined the classical period as the minimal period of the Hessian $h''(X_t)$ which is not necessarily the period of the classical flow Φ_h^t. An example is classical unbounded motion in a one dimensional periodic potential V_Γ with energies E such that

$$E > \sup_{x \in \mathbb{R}} (V_\Gamma(x)).$$

In such a case $h''(X_t)$ is periodic although the flow $\Phi_h^t(X_0)$ is not. Furthermore, the approximation remains localized between classical periods if

$$\varkappa = 2T \sup_{t \in [0,T]} \left\| \mathscr{J} h''(X_t) \right\|_{\mathrm{HS}},$$

the exponent in (4.57), is small enough. We can hence state in that case, up to small errors $\mathcal{O}(\hbar^{\alpha})$, localization of the exact propagation up to the Ehrenfest time $T_E \propto \hbar^{-\frac{1}{2}}$.

4.6 Bohr–Sommerfeld quantization conditions

Of particular importance in quantum mechanics are the spectral properties of operators and foremost Hamiltonian operators. We seek here approximations to eigenvalues of a Hamiltonian $\widehat{h}$ through quasi–modes. A quasi–mode satisfies the spectral problem up to a discrepancy δ, i.e., a quasi–mode ψ_E is a $\delta-$approximate solution with energy E,

$$\left\| \left(\widehat{h} - E\right) \psi_E \right\| \leq \delta. \tag{4.72}$$

If the spectrum is discrete, this ensures that there is an eigenvalue $\mathscr{E}_i$ of $\widehat{h}$ in the interval $[E-\delta, E+\delta]$ (see, e.g., [Laz93]). Note that ψ_E is not necessarily close to an eigenfunction. A simple illustration is given if $\mathscr{E}_i$ is nearly degenerate in which case it is clear that any linear combination of true eigenfunctions is a good quasi–mode. These linear combinations are, in general, not good approximations of the eigenfunctions.

Up to now, we have used the properties of Gaußians to introduce semiclassical approximations. We will here continue with a description of a construction devised by Paul and Uribe [PU93]. Our goal is to introduce the well known Bohr-Sommerfeld quantization conditions.

It is clear from section 4.3.3 that for some $X_0 \in \mathbb{R}^2$ such that $h(X_0) = E$, $\psi_{X_0}^{Z_0}$, $(Z_0 \in \Sigma_d)$ is an $\hbar^{\frac{1}{2}}-$quasi–mode. It is generally a highly degenerate one since any point $X \in h^{-1}(E)$ chosen on a classical path also is a quasi–mode at this energy. Paul and Uribe [PU93] constructed quasi–modes using the ansatz

$$\psi_{\Lambda(E)} = \int_0^T \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Et} \mathscr{U}(t) \psi_{X_0}^{Z_0} \, \mathrm{d}t. \tag{4.73}$$

To illustrate this, we compute

$$\begin{aligned}
\left(\widehat{h} - E\right) \psi_{\lambda(E)} &= \int_0^T \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Et} \left(\widehat{h} - E\right) \mathscr{U}(t) \psi_{X_0}^{Z_0} \, \mathrm{d}t && (4.74)\\
&= \int_0^T \mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} \left(\mathrm{e}^{\frac{\mathrm{i}}{\hbar}Et} \mathscr{U}(t) \psi_{X_0}^{Z_0} \right) \mathrm{d}t && (4.75)\\
&= \mathrm{i}\hbar \left(\mathrm{e}^{\frac{\mathrm{i}}{\hbar}ET} \mathscr{U}(T) \psi_{X_0}^{Z_0} - \psi_{X_0}^{Z_0} \right). && (4.76)
\end{aligned}$$

Now, assume

$$\varkappa = \sup_{\tau\in[0,T]} \left(h''(X_\tau)\right) \tag{4.77}$$

is small enough. We then have

$$\left(\widehat{h} - E\right)\psi_{\Lambda(E)} = \mathrm{i}\hbar\left(\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(ET+\Theta(T))} - 1\right)\psi_{X_0}^{Z_0} + \mathcal{O}\left(\hbar^{\frac{3}{2}}\right) \tag{4.78}$$

if $\psi_{X_0}^{Z_0}$ has a classical revival at T. This is only possible if the corresponding Floquet matrix is diagonalizable and the exponents are purely imaginary according to Theorem 4.3.

On the other hand, one has to require

$$ET + \Theta(T) = 2\pi\hbar n, \quad n \in \mathbb{Z}, \tag{4.79}$$

(we use the notation of section 4.3.2) in order to obtain

$$\left\|\left(\widehat{h} - E\right)\psi_{\Lambda(E)}\right\| = \mathcal{O}\left(\hbar^{\frac{3}{2}}\right), \tag{4.80}$$

then $\psi_{\Lambda(E)}$ is a $\hbar^{\frac{3}{2}}-$quasi–mode.

In other words, the Bohr-Sommerfeld quantization condition

$$\mathcal{S}_{\Lambda(E)} = 2\pi\hbar\left(n + \frac{\mu}{4}\right) \tag{4.81}$$

produces approximate eigenvalues $\mathcal{E}_n(\hbar)$ to a countable set of integral curves with energies $\mathcal{E}_n(\hbar)$ in $\mathrm{T}^*\mathbb{R}^d$. This implies that true eigenvalues of $\widehat{h}$ lie in the intervals $I_n \cong \left[E_n - C_n\hbar^{\frac{3}{2}}, E_n + C_n\hbar^{\frac{3}{2}}\right]$, where $C_n > 0$ is $\hbar-$independent. Since for a $d-$dimensional system, the mean separation between eigenvalues is $\mathcal{O}\left(\hbar^{d-1}\right)$ [Ivr84], these quasi–modes only produce useful information in the case $d \leq 2$.

The quasi–modes we have developed here have an important property: they are, as we shall see, not singular in contrast to WKB wave functions.

4.7 WKB

Here we introduce the WBK approximation. In the physical literature this is attributed to G. Wentzel, A. Kramers and L. Brillouin. More recently this theory has been attacked in a more geometrical manner [Hör71, MF81, Vor76]. We present it here for a one dimensional system. In the next section, we show that

this construction can be extended under certain assumptions to $d-$dimensional systems.

The main idea is to find approximate solutions to the time independent Schrödinger equation

$$E\psi(x) = -\frac{\hbar^2}{2}\Delta_x\psi(x) + V(x)\psi(x) \tag{4.82}$$

with energy E using the standard WKB ansatz

$$\psi = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi(x)} \sum_{i\in\mathbb{N}_0} \hbar^i a_i(x). \tag{4.83}$$

By insertion into (4.82), one finds that

$$\psi_{\mathrm{WKB}}(x) = a_0(x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi(x)} + \mathcal{O}(\hbar) \tag{4.84}$$

will be an approximate solution, if $\phi(x)$ satisfies

$$H\left(\frac{\partial\phi}{\partial x}, x\right) = E, \tag{4.85}$$

where $H(p,q) = \frac{p^2}{2} + V(q)$ is the corresponding classical Hamiltonian. This means that $\phi(x) = \mathcal{S}(x,E)$ where

$$\mathcal{S}(x,E) = \int_{x_0}^{x} p(q,E)\,\mathrm{d}q - \mathcal{S}_0 \tag{4.86}$$

is the reduced action along the classical trajectories corresponding to H with energy E (see section 3). The constant $\mathcal{S}_0$ is arbitrary since only the derivative of $\mathcal{S}$ enter the condition (4.85). This term only constitutes an overall phase to the WKB ansatz. We will suppress this term since we are mostly interested with the spatial changes of the reduced action and not the actual value of the phase $\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathcal{S}(x)}$.

Furthermore, a_0 must satisfy the continuity equation

$$\frac{\partial\mathcal{S}(x)}{\partial x}\frac{\partial a_0(x)}{\partial x} + \frac{1}{2}\frac{\partial^2\mathcal{S}(x)}{\partial x^2}a_0(x) = 0 \tag{4.87}$$

usually called transport equation due to its form. Its solution can be written more explicitly as

$$a_0(x) = \left(\frac{\partial\mathcal{S}}{\partial x}\right)^{-\frac{1}{2}} = \frac{1}{\sqrt{|p(x)|}}, \tag{4.88}$$

where p is the classical momentum generated by $\mathscr{S}$. It is possible to collect all terms in powers of $\hbar$. Demanding that each such term of power $i \in \mathbb{N}$ vanishes, one finds

$$\frac{\partial \mathscr{S}(x)}{\partial x}\frac{\partial a_i(x)}{\partial x} + \frac{1}{2}\frac{\partial^2 \mathscr{S}(x)}{\partial x^2}a_i(x) = \frac{\mathrm{i}}{2}a_{i-1}(x). \tag{4.89}$$

If it is possible to recursively solve for a_i, one has then an asymptotic solution to $\mathscr{O}(\hbar^\infty)$ to the spectral problem of (4.82). We wish to note here that additional terms appear in the recursion if the sub–principal symbols of the considered operator do not vanish such as in this case. Note that here, again, the constant $\mathscr{S}_0$ does not play a role since only derivatives of $\mathscr{S}(x)$ enter.

For our purposes, it will suffice to consider

$$\psi_{\mathrm{WKB}}(x) = \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathscr{S}(x)}}{\sqrt{|p(x)|}} + \mathscr{O}(\hbar). \tag{4.90}$$

Obviously, the above WKB approximation has a rather awkward property at the classical turning points of the classical trajectories since it diverges there. In general ψ_{WKB} is hence not in $\mathrm{L}^2(\mathbb{R})$. Two remedies have so far been devised. Both make use of more or less advanced "cut and paste techniques" to avoid such divergences. The older method uses a linearization of the potential around the classical turning point. This uses the properties of the Airy function as solution of the linearized equation. The Airy function is asymptotically oscillatory in one direction and exponential in the other. This allows to construct a bounded approximate solution which is exponentially decreasing in the classically forbidden region $\{x : V(x) > E\}$ and oscillating in the classically allowed region. WKB wave functions for bound states are then constructed by a careful composition of the different approximations around and beyond the turning points by considering so called Stokes multipliers [BM72]. Demanding single-valuedness of the WKB wave function usually gives additional constraints. These usually describe approximate eigenvalues as they emerge, e.g., from the Bohr-Sommerfeld quantization conditions.

The second approach is based on the fact that the existence of the above singularities is related to the parameterization of the WKB approximation. Such results were introduced by Maslov and Hörmander amongst others. We refer to [Hör71, MF81] for a complete account. We will here introduce the result in a less abstract manner. We start by remarking that the above construction can be made locally. We see a classical path as a purely geometric object. By the Lemma 3.1 there always exists a function that at least locally generates a Lagrangian manifold. In practice we first define charts, i.e., bijections

$$(\xi_\alpha, x_\alpha) \quad : \quad U_\alpha \to D_\alpha$$

$$m \mapsto \left(\xi_{\alpha,1}(m), ..., \xi_{\alpha,N}(m), x_{\alpha,1}(m), ..., x_{\alpha,N}(m)\right)$$

from subsets U_α of a manifold M to open subsets D_α of $\mathbb{R}^N$ (here $\mathbb{R}^2$). We assume from now on that such a choice of sets U_α covers the manifold, i.e., $M = \bigcup_\alpha U_\alpha$. We can freely choose to write our ansatz as a function in momentum or position, i.e., we can find a collection of charts, an atlas of local charts, such that we may describe the classical trajectory on such a chart either by $\left(\frac{\partial \mathscr{S}}{\partial x}, x\right)$ or $\left(\xi, \frac{\partial \mathscr{W}}{\partial \xi}\right)$. The word "locally" just means that we only consider objects on a specific neighborhood U_α. This means in our case that the WKB ansatz is to be considered in a specific form on a specific chart. Formally an ansatz in momentum parametrization can be constructed in a similar way as that of the above ansatz in position. This representation will not be singular at the turning points. Each local construction is a solution of the spectral problem up to $\mathscr{O}(\hbar)$.

In order to construct a global solution, we must join the different local representations in an acceptable way. Since the representations were chosen in position and momentum respectively, one is then led to investigate Fourier integrals of the type

$$\left(\mathscr{F}_\hbar \psi_{\mathrm{WKB}}\right)(\xi) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\mathscr{S}(x) - \xi x)}}{\sqrt{|p(x)|}} + \mathscr{O}(\hbar)\,\mathrm{d}x. \tag{4.91}$$

These can be treated as oscillatory integrals. The leading contribution to the integral, according to the stationary phase theorem (see, e.g., [DS99]), is given by the points for which the derivative of $\mathscr{W} = \mathscr{S}(x) - x\xi$ vanishes. These are simply given by the classical path $(\xi, q(\xi))$ corresponding to the energy E. We denote by $\mathrm{sgn}(Q)$ the number of negative eigenvalues of the matrix Q. Insertion yields

$$\left(\mathscr{F}_\hbar \psi_{\mathrm{WKB}}\right)(\xi) = \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\mathscr{W}(\xi) - \frac{\mathrm{i}\pi}{2}\mathrm{sgn}\left(\mathscr{S}''(q(\xi))\right)}}{\sqrt{\left|p(q(\xi))p'(q(\xi))\right|}} + \mathscr{O}(\hbar) \tag{4.92}$$

which is non-singular as long as the derivative of the potential does not vanish. Note that the phase term $\mathrm{e}^{-\frac{\mathrm{i}\pi}{4}\mathrm{sgn}\left(\mathscr{S}''(q(\xi))\right)}$ is related to the Hessian $\mathscr{S}''$ of the classical action (which is equal to the Hessian of $\mathscr{W}$).

Of particular interest are hence the points where the eigenvalues of the Hessian $\mathscr{S}''$ changes sign. Such points are generally caustics of the classical motion. Here they are simply the classical turning points if we disregard certain situations such as unstable fixed points of the Hamiltonian flow.

We consider now the changes in the additional phase along the classical path. To do this, we assume to have an atlas of charts that cover the classical path. Charts where the position representation are singular will be called singular

charts. The others will be called non-singular ones. We further assume, for simplicity, that we cover the classical path with a minimum number of charts, namely, twice the number of singular points along the classical path, such that the supports U_α of two neighboring charts intersect in one point (see figure 4.1).

The approximation will be described locally in either momentum representation for singular charts or in position representation for non–singular charts. We wish to associate to each chart a natural number μ such that the additional phase above is given by $e^{-i\frac{\pi\mu}{4}}$. Progressing along the classical path (in the direction given by the classical motion), one has to change the representation in the vicinity of a singular points. For one dimensional systems, the position representation will be singular at the turning points. In momentum representation the singular points will be given by the local extrema of the potential. Each time a singular point is passed, the WKB ansatz gains a phase given by (4.92) from a chart α with coordinates (p_α, q_α) to the passage to the next chart β with coordinates $\left(p_\beta, q_\beta\right)$ according to

$$\Delta\mu = \operatorname{sgn}\left(\mathscr{S}''\left(p_\beta, q_\beta\right)\right) - \operatorname{sgn}\left(\mathscr{S}''(p_\alpha, q_\alpha)\right). \tag{4.93}$$

Such a construction does not define the phases in a unique way since there resides some ambiguity in the choices of the charts, initial point and initial phase. However, with a specific choice of charts, each chart can be assigned natural numbers defined for the chart by incrementation according to (4.93). What will be important to us is the actual phase difference of the ansatz after one revolution around the classical trajectory. This phase difference is defined in a unique manner by the above construction, i.e., this phase is invariant on the choice of charts. For closed classical trajectory in a 2 dimensional phase space, this phase change given by $\mu = 2$ (see figure 4.1). It is integer–valued for closed loops.

Such numbers, μ, are called Maslov indices. They appear in a similar manner in higher dimensions as here, i.e., as the number of negative eigenvalues of the Hessian of $\mathscr{S}$. Contrarily to the one dimensional case, this Hessian is a $2d \times 2d$ matrix and the Maslov index is incremented each time one of the eigenvalues of the Hessian changes sign. Note further that the Maslov index needs only to be defined modulo four. It will be a natural number for closed loops.

The benefit of such a construction is that the earlier quantization constraints on ψ_{WKB} now gives $\hbar^2-$quasi–modes. Single valuedness after one revolution on the classical path gives the corrected Bohr-Sommerfeld quantization condition [Kel58]

$$\oint_{\Lambda(E)} p\,\mathrm{d}q = 2\pi\hbar\left(n + \frac{\mu}{4}\right), \quad n \in \mathbb{N}, \tag{4.94}$$

where μ is the Maslov index of the classical trajectory $\Lambda(E)$ of energy E.

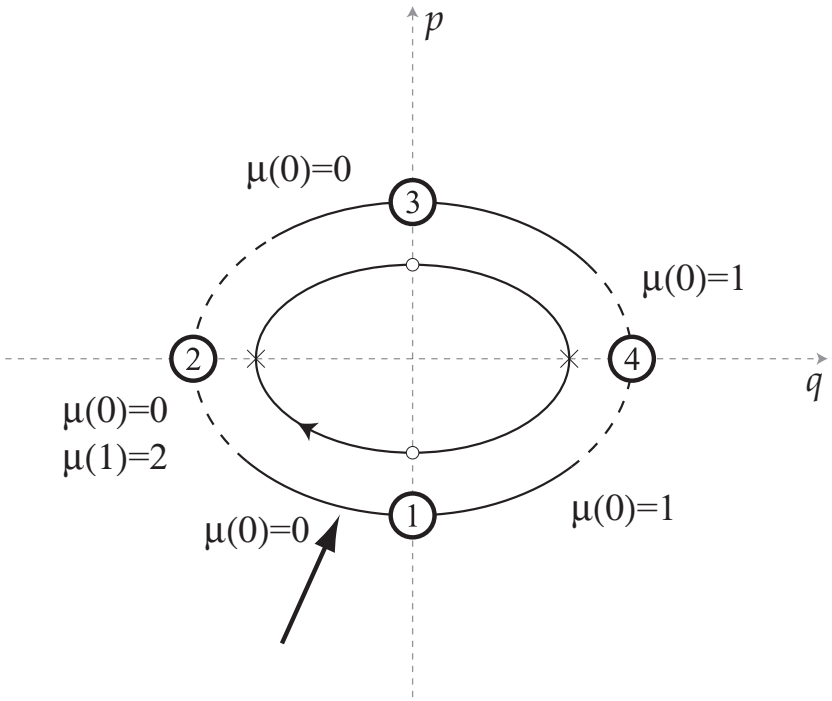

Figure 4.1: A diagram of the sectors defined by an atlas of the local charts necessary to construct a WKB ansatz globally. Here, we consider the simplest case of a one dimensional closed classical path, i.e., the classical motion is periodic around a single minimum at $q = 0$ of the classical potential. The loop in the center represents the classical path in phase space where the singular points are marked out. The local extrema of the potential (minimum) are marked with white circles whereas the turning points are marked with crosses. The four numerated elliptic arcs outside represent the sectors covered by the different charts. The chart with representations in momentum are dashed while position representations are full lines. Each sector is given with its index $\mu(i)$ as constructed which has to be incremented when the derivative of the momentum changes sign since for a one dimensional system $\frac{\partial^2 \mathcal{S}(x)}{\partial x^2} = p'(x)$. The index i in parenthesis tracks the number of revolutions around the trajectory. The construction is started at the arrow. When one revolution is completed, one notices that the WKB ansatz has acquired a phase difference to the original WKB ansatz (to sector 1 we have the initial $\mu(0) = 0$ marked and the value after one revolution $\mu(1) = 2$). Demanding single valuedness of the WKB ansatz gives a corrected Bohr-Sommerfeld quantization.

4.8 EBK quantization

In one dimension, the Bohr–Sommerfeld quantization condition emerges as a consequence of the single valuedness of the WKB ansatz. To do this, we used closed classical trajectories. Such trajectories always exist for one dimensional bounded classical motion since one dimensional systems are always integrable, i.e., the level set of constant energy E in phase space consists of closed curves.

In d dimensions, it is still possible to formulate a quantization procedure if the system is integrable, i.e., if the system satisfies the integrability conditions of Theorem 3.3. Classical systems which satisfy the requirements of this theorem are equivalent to d linear independent motions on a (Liouville–Arnold) d dimensional torus M_α. It is invariant under the flows $\Phi_i^{t_i}$ corresponding to the d functions A_i that are in involution (we refer to the notation of Theorem 3.3). The different flows $\Phi_i^{t_i}$ commute. We can associate WKB ansätze for the operators $\mathrm{Op}_\hbar^{\mathrm{w}}\left[A_i\right]$ along flow lines of $\Phi_i^{t_i}(\xi, x)$ parametrized in a similar way as the above ansatz in one dimensional systems. More generally one considers a product of d such WKB ansätze, one for each A_i. Such an ansatz is still associated to an energy E since the corresponding action generates level sets in $\lambda^{-1}(E)$. More precisely, the action

$$\mathscr{S}(x) = \int_{x_0}^{x} p \, \mathrm{d}q \tag{4.95}$$

along the flow lines $\Phi_1^{t_1} \circ \ldots \circ \Phi_d^{t_d}(\xi_0, x_0)$ satisfies the Hamilton–Jacobi equation (4.85), i.e., $\mathrm{Op}_\hbar^{\mathrm{w}}[H]\,\psi_{\mathrm{WKB}}$ is $E\psi_{\mathrm{WKB}}$ up to $\mathscr{O}(\hbar^\infty)$ where we assume the full ansatz (4.83). In particular, the flows $\Phi_i^{t_i}$ commute and the composite flow $\Phi_1^{t_1} \circ \ldots \circ \Phi_d^{t_d}$ covers M_α when parametrized by $t_1, \ldots, t_d$. This means that the composite flow can describe any trajectory on M_α. Since we will, again, use the single valuedness of the WKB ansatz we will consider any such closed trajectories on M_α.

The Liouville–Arnold torus can be given a basis of d simple loops $\mathscr{C}_i$. We choose here the cycles corresponding to the d tori described by the d independent motions of Theorem 3.3. The suitable coordinates are the action–angle variables $(\mathscr{I}_i, \varphi_i)$ where $\mathscr{I}_i$ is the action corresponding to a loop $\mathscr{C}_i$ and φ_i the corresponding angle (see section 3.4). According to the previous paragraph, we may consider any closed trajectory on M_α described by $\Phi_1^{t_1} \circ \ldots \circ \Phi_d^{t_d}(\xi, x)$, i.e., we consider any closed loop around M_α. Since M_α is Lagrangian, the actions corresponding to continuous deformations of loops are equal. We may hence restrict our study to the corresponding equivalence classes of loops. These simply correspond to the linear combinations of the cycles $\mathscr{C}_i$.

Practically this means that we can write a product WKB ansatz where each

term corresponds to a loop $\mathscr{C}_i$ and a corresponding winding number w_i, i.e., the number of times the loop $\mathscr{C}_i$ is repeated along the trajectory. Particularly, the motion along a full cycle $\mathscr{C}_i$ will contribute with a phase

$$\mathrm{e}^{2\pi \mathrm{i} w_i \frac{\mathscr{I}_i}{\hbar}}, \tag{4.96}$$

to the WKB ansatz.

Naturally, the Maslov construction must also be taken into account. To each simple loop $\mathscr{C}_i$ we define a Maslov index μ_i. We note that the Maslov index can be shown to be an invariant for each of the above equivalence classes of loops. Each loop will then contribute with a phase factor

$$\mathrm{e}^{2\pi \mathrm{i} w_i \left(\frac{\mathscr{I}_i}{\hbar} - \frac{\pi \mu_i}{4}\right)}. \tag{4.97}$$

Hence, each $\mathscr{C}_i$ will independently result in a Bohr–Sommerfeld like quantization condition

$$\mathscr{I}_i = \hbar\left(n_i + \frac{\mu_i}{4}\right), \quad n_i \in \mathbb{Z} \tag{4.98}$$

when demanding single valuedness of the WKB ansatz. Note the winding number w_i does no longer enter the expression since the cases when $w_i \neq 1$ are automatically treated when $n_i \in \mathbb{Z}$. The full quantization condition is then the collection of the d conditions originating from the d independent flows. In this form, the quantization procedure is then called EBK–quantization[4]. This was first formulated fully by Keller [Kel58].

In the integrable case, the quantization reduces to d one dimensional quantizations. One notes further that the actions $\mathscr{I}_i$ are invariant under symplectomorphism. In this way one retrieves the quantization condition we found previously for one dimensional systems. The missing factor 2π in (4.98) is merely a consequence of the normalization of $\mathscr{I}_i$, i.e.,

$$\mathscr{I}_i = \frac{1}{2\pi} \oint_{\mathscr{C}_i} p \, \mathrm{d}q. \tag{4.99}$$

[4]The abbreviation stands for A. Einstein, L. Brillouin and J. Keller

Chapter 5

Perturbation of periodic operators

We focus our attention on periodic systems and their perturbations. Such systems have been extensively studied, partly due to their applications in solid state physics. One considers in this case the effective potential created by individual atoms acting on a particle, e.g., an electron. These atoms are assumed to be arranged in a regular lattice which generate the periodicity of the potential. More recent but equivalent systems are those with particles trapped in optical lattices. In this case, the periodic potentials arise from the action of lasers. These are arranged such that the lasers produce standing waves which create periodic electro-magnetic potentials.

We have already studied the spectral properties of such systems in the first chapter (under the name Hill equation). We will adopt a slightly different, but equivalent, approach in this chapter for the purely periodic case. Our main aim is the description of the spectrum of such operators under perturbations. It is known under fairly general assumptions that the spectrum remains absolutely continuous under perturbations [CH91, Sob99].

The perturbation of such operators also has a long history. Already Bloch [Blo28] foresaw that electrons in a crystal under the action of an electric potential would start to oscillate (Bloch oscillations). Later, it was foreseen that resonances would emerge aligned in so–called Wannier–Stark ladders [Wan60, Wan62, WF62].

Peierls proposed a semiclassical approach to the treatment of the dynamics of such problems. He suggested that one should be able to substitute the periodic part of the Schrödinger operator by an appropriate dispersion relation[1].

The main ingredient of such results is an adiabatic decoupling. One considers the effective dynamics described classically by some of the degrees of freedom and the remaining degrees of freedom are described quantum mechanically.

[1]This substitution is known as Peierls or Peierls–Onsager substitution.

Typically the degrees of freedom described classically are varying much slower than those described quantum mechanically. The quantum degrees of freedom are considered to have quantized energy eigenvalues for a given configuration of the classical degrees of freedom. The quantized energies are further assumed to vary continuously when the classical degrees of freedom are altered. Projecting the values of one energy eigenvalue for all possible classical configurations, one acquires an energy band. In such a case, adiabatic decoupling then resides in the approximation that the slow varying degrees of freedom will not alter significantly the system, i.e., the quantum degrees of freedom will remain in a given energy band although the slow changing degrees of freedom are altered. One then describes the dynamics of the system as the dynamics by the classical mechanics generated by an eigenvalue band of the Hamiltonian. Higher order corrections include the effects of neighboring bands. Celebrated examples include the Foldy–Wouthuysen effective description of a relativistic fermion, the Born–Oppenheimer approximation of nuclear–electronic motions, the Peierls–Onsager substitution in solid state physics and the Bohr–Mottelsson description of rotating nuclei.

To ensure a clear presentation, we assume $\hbar = 1$. Asymptotic considerations will be conducted in the parameter ε (to be introduced below).

5.1 Periodic Schrödinger operators

5.1.1 The Bloch–Floquet transform

The goal here is to study spectral properties of the periodic Schrödinger operator

$$\widehat{H}_\Gamma := \frac{\widehat{p}^2}{2} + V_\Gamma(x) \tag{5.1}$$

acting on $\mathrm{L}^2\left(\mathbb{R}^d\right)$, where V_Γ is bounded and periodic with respect to a lattice $\Gamma \cong \mathbb{Z}^d$. $\mathscr{M} \cong \mathbb{R}^d/\Gamma \cong \mathbb{T}^d$ is the fundamental cell of the Bravais lattice Γ and $\mathscr{M}^*$ is the fundamental cell of Γ^*, that is, the first Brillouin zone. We will identify the fundamental cell with the central fundamental cell,

$$\mathscr{M} = \left\{ x \in \mathbb{R}^d : x = \sum_{i=1}^{d} \xi_i \gamma_i,\ \xi_i \in \left[-\frac{1}{2}; \frac{1}{2} \right] \right\} \tag{5.2}$$

where $\{\gamma_1, \gamma_2, \ldots \gamma_d\}$ is a lattice basis such that

$$\Gamma = \mathbb{Z}\gamma_1 \oplus \mathbb{Z}\gamma_2 \oplus \ldots \oplus \mathbb{Z}\gamma_d. \tag{5.3}$$

The first Brillouin zone $\mathscr{M}^*$ is identified analogously. The lattice Γ^* is generated by the dual lattice basis $\{\gamma_1^*, \gamma_2^*, ...\gamma_d^*\}$ that satisfies $\gamma_i \cdot \gamma_j^* = 2\pi\delta_{ij}$.

The main tool here will be the Bloch–Floquet transform. We will basically follow the description of [PST03]. The Bloch–Floquet transform is the isomorphism

$$\begin{aligned} \mathscr{U}_{\mathrm{BF}} \quad : \quad & \mathrm{L}^2\left(\mathbb{R}^d\right) \to \mathscr{H}_\tau \\ & \Psi(x) \mapsto \psi(k, y), \end{aligned} \tag{5.4}$$

where $\mathscr{H}_\tau$ is the space of locally square integrable functions which transform in a certain way under Brillouin lattice translations. For fixed k, these function have values in $\mathrm{L}^2(\mathscr{M})$, namely, they are in

$$\mathscr{H}_\tau \cong \{\psi(k, y) \in \mathrm{L}^2_{\mathrm{loc}}\left(\mathbb{R}^d, \mathrm{L}^2(\mathscr{M})\right) : \psi(k - \gamma^*) = \tau(\gamma^*)\psi(k)\}. \tag{5.5}$$

$\mathscr{H}_\tau$ is a Hilbert space with the inner product

$$\langle \psi | \phi \rangle = \int_{\mathscr{M}^*} \langle \psi(k) | \phi(k) \rangle_{\mathrm{L}^2(\mathscr{M})} \, \mathrm{d}k. \tag{5.6}$$

The fact that these function gain a phase when translated by one dual lattice spacing can be introduced by the unitary representation τ of the group of lattice translations on Γ^*. We have thus

$$\tau \quad : \quad \Gamma^* \to \mathscr{B}\left(\mathrm{L}^2(\mathscr{M}^*)\right) \tag{5.7}$$

$$\gamma^* \to \tau(\gamma^*), \forall \gamma^* \in \Gamma^*, \tag{5.8}$$

with eigenvalues $\mathrm{e}^{\mathrm{i}y\cdot\gamma^*}$,

$$\tau(\gamma^*)\psi(y) = \mathrm{e}^{\mathrm{i}y\cdot\gamma^*}\psi(y). \tag{5.9}$$

Note that with the trivial representation $\mathscr{H}_\tau$ is nothing else than

$$\mathscr{H}_{\tau=1} \cong \{\psi \in \mathrm{L}^2_{\mathrm{loc}}\left(\mathbb{R}^d, \mathrm{L}^2(\mathscr{M})\right) : \psi(k - \gamma^*) = \psi(k)\}, \tag{5.10}$$

that is, the space of Γ^*-periodic functions

$$\mathscr{H}_{\tau=1} \cong \ell^2\left(\mathbb{Z}^d\right) \otimes \mathrm{L}^2(\mathscr{M}) \cong \mathrm{L}^2(\mathscr{M}^*) \otimes \mathrm{L}^2(\mathscr{M}). \tag{5.11}$$

The last step is to be seen as the unitary equivalence between the Fourier series on $\mathscr{M}$ and the $\Gamma-$periodic functions on $\mathbb{R}^d$. Similarly, the identification can be made with $\mathscr{H}_\tau$ by restriction of $\mathbb{R}^d$ to $\mathscr{M}^*$. This identification is uniquely

determined by extending the functions in $\mathrm{L}^2(\mathscr{M}^*) \otimes \mathrm{L}^2(\mathscr{M})$ $\tau-$equivariantly, i.e., such that they satisfy

$$\psi(k-\gamma^*) = \tau(\gamma^*)\psi(k). \tag{5.12}$$

We can hence identify $\mathscr{H}_\tau$ in the following way

$$\mathscr{H}_\tau \cong \mathrm{L}^2(\mathscr{M}^*) \otimes \mathrm{L}^2(\mathscr{M}). \tag{5.13}$$

The functions in $\mathscr{H}_\tau$ satisfy

$$\begin{aligned} \psi(k-\gamma^*, y) &= \mathrm{e}^{\mathrm{i}\gamma^* y}\psi(k,y), \forall \gamma^* \in \Gamma^*, \\ \psi(k, y+\gamma) &= \psi(k,y), \forall \gamma \in \Gamma. \end{aligned} \tag{5.14}$$

Defining the Bloch Floquet transform as

$$\mathscr{U}_{\mathrm{BF}}\psi(y) = \sum_{\gamma\in\Gamma} \mathrm{e}^{\mathrm{i}(y+\gamma)\cdot k}\psi(y+\gamma), y \in \mathbb{R}^d, \tag{5.15}$$

$$\mathscr{U}_{\mathrm{BF}}^{-1}\psi(k,[x]) = \int_{\mathscr{M}^*} \mathrm{e}^{\mathrm{i}k\cdot x}\psi(k,[x])\,\mathrm{d}k, \tag{5.16}$$

the above properties can be checked, e.g., if $\psi \in \mathrm{L}^2\left(\mathbb{R}^d\right)$ we have $\mathscr{U}_{\mathrm{BF}}\psi \in \mathscr{H}_\tau$. We denote here by $[x] \in \mathscr{M}$ the unique decomposition of $x \in \mathbb{R}^d$

$$x \stackrel{\mathrm{def}}{=} [x] + \gamma, \quad \gamma \in \Gamma, \tag{5.17}$$

where γ is chosen "maximal".

Furthermore, $\mathscr{H}_\tau$ can be seen as the (constant) fiber decomposition of

$$\mathscr{U}_{\mathrm{BF}}\mathrm{L}^2\left(\mathbb{R}^d\right), \tag{5.18}$$

i.e.,

$$\mathscr{H}_\tau = \int_{\mathscr{M}^*}^{\oplus} \mathscr{H}(k)\,\mathrm{d}k, \tag{5.19}$$

with $\mathscr{H}(k) \cong \mathrm{L}^2(\mathscr{M})$. Moreover, we have

$$\mathscr{U}_{\mathrm{BF}}^{-1}\widehat{H}_\Gamma\mathscr{U}_{\mathrm{BF}} = \int_{\mathscr{M}^*}^{\oplus} \widehat{H}_{\mathrm{BF}}(k)\,\mathrm{d}k. \tag{5.20}$$

Of particular importance is the fact that $\widehat{H}_{\mathrm{BF}}(k)$ can be written as

$$\widehat{H}_{\mathrm{BF}} = \frac{1}{2}\left(-\mathrm{i}\nabla_y^{\mathrm{per}} + k\right)^2 + V_\Gamma(y), \tag{5.21}$$

where ∇_y^{per} is the gradient with periodic boundary conditions as (5.14) indicates. We will not elaborate on the last statement which requires some more precise discussions of the domains of the included operators (see [PST03] and references therein). In essence, we can see the Bloch–Floquet transform of the position and momentum operators as

$$\mathcal{U}_{\text{BF}}^{-1}\widehat{p}\,\mathcal{U}_{\text{BF}} = \mathbb{1}\otimes\left(-\mathrm{i}\nabla_y\right) + k\otimes\mathbb{1}, \tag{5.22}$$

$$\mathcal{U}_{\text{BF}}^{-1}\widehat{x}\,\mathcal{U}_{\text{BF}} = \mathrm{i}\nabla_k^{\tau}, \tag{5.23}$$

with dense domains in $\mathscr{H}_\tau$. ∇_k^τ is the gradient with respect to k with τ–equivariant conditions according to (5.14).

5.1.2 An equivalent approach

We started this thesis by considering the Hill equation. At this point, we would like to stress that the spectral problem associated with $\widehat{H}_\Gamma$ is reduced to the Hill equation

$$\left(-\mathrm{i}\nabla_x\right)^2\psi + 2(-E+V_\Gamma)\psi = 0. \tag{5.24}$$

We assume $d=1$ henceforth and that the lattice spacing is 2π. With this in mind, we proceed by studying the Bloch–Floquet transform of $\widehat{H}_\Gamma$, $\widehat{H}_{\text{BF}} : \mathscr{H}_\tau \to \mathscr{H}_\tau$. Note that we can view $\mathscr{H}_\tau$ as $\mathrm{L}^2(\mathscr{M}^*)\otimes\mathrm{L}^2(\mathscr{M})$, hence, for fixed k we can see $\widehat{H}_{\text{BF}}(k)$ as $\widehat{H}_{\text{BF}}(k) : \mathrm{L}^2(\mathscr{M}) \to \mathrm{L}^2(\mathscr{M})$. We can hence, without loss of generality, assume an ansatz

$$\psi(k,y) = \mathrm{e}^{\mathrm{i}k\cdot y}\sum_{i\in\mathbb{Z}} c_i \mathrm{e}^{\mathrm{i}j\cdot y}, \tag{5.25}$$

which inserted in (5.24) leads to

$$c_j + \frac{q}{(2k-n)^2 - E}\left(c_{j+1}+c_{j-1}\right) = 0. \tag{5.26}$$

We have assumed a one dimensional system with $V_\Gamma(y) = q\cos(y)$ to illustrate this. This is exactly what we would have found with the approach of the first chapter. There is, however, one distinction: we now seek solutions in $\mathscr{H}_\tau$ and not in $\mathrm{C}^2\left(\mathbb{R}^d\right)\otimes\ell^2(\mathbb{Z})$ as previously. This excludes all solutions which have a Floquet exponent with non-vanishing real part. At this point we see that k is none other than the imaginary part of the above defined (purely imaginary) Floquet exponents. It is usually called quasi–momentum.

We can hence only allow solutions with purely imaginary Floquet exponents. As discussed before, the results of Lyapunov [Lia07] ensures us that the

spectrum of $\widehat{H}_{\mathrm{BF}}$ occurs in bands. Furthermore, it can be shown that $\widehat{H}_{\mathrm{BF}}(k)$ is essentially self-adjoint on $\mathscr{H}(k)$ and has purely discrete spectrum with eigenvalues $\mathscr{E}_n(k)$, see [RS78]. We also state the following for future use.

Theorem 5.1. *Suppose V_Γ is piecewise continuous with period 2π. Then:*

1. *$\widehat{h}(k)$ has purely discrete spectrum and is real analytic in k.*
2. *$\widehat{h}(k)$ and $\widehat{h}(2\pi - k)$ are anti-unitarily equivalent under ordinary complex conjugation. In particular, their eigenvalues are identical and their eigenfunctions are complex conjugates.*
3. *For $k \in (0, \pi)$, or in $(\pi, 2\pi)$, $\widehat{h}(k)$ has only non degenerate eigenvalues.*
4. *Let $\mathscr{E}_n(k)$, $(n = 0, 1, ...; 0 \leq k \leq \pi)$ denote the nth eigenvalue. Then each $\mathscr{E}_n(\cdot)$ is analytic in $(0, \pi)$ and continuous at $k = 0$ and π.*
5. *For n odd (respectively, even) $\mathscr{E}_n(k)$ is strictly monotonously increasing (respectively decreasing) as k increases from 0 to π. In particular*

$$\mathscr{E}_1(0) < \mathscr{E}_1(\pi) \leq \mathscr{E}_2(\pi) < \mathscr{E}_2(0) ... \leq \mathscr{E}_{2n-1}(0) < \mathscr{E}_{2n-1}(\pi) \leq \mathscr{E}_{2n}(\pi) < ...$$

This theorem can be found in [RS78] as well as the proof. This type of results cannot in general be given in arbitrary dimension because of possible eigenvalue crossings and other phenomena generated by higher dimensions.

To this, we add another classical result, namely, the fact that $\widehat{H}_\Gamma$ has absolutely continuous spectrum in bands [Tho73]. This is also true for magnetic potentials, i.e., replacing $-\mathrm{i}\nabla_x$ by $\left(-\mathrm{i}\nabla_x - \mathscr{A}(x)\right)$ where $\mathscr{A}$ is a magnetic vector potential that is small enough [HH95, Sob99].

5.1.3 $\tau-$equivariant symbols

In section 4.1 we introduced the Weyl quantization of operator valued symbols on $\mathrm{T}^*\mathbb{R}^d$. This scheme can also be extended to operator valued symbols on $\mathrm{T}^*\mathbb{T}^d$ or a $\tau-$equivariant operator valued symbols [PST03, GN98]. Notice that the semiclassical parameter is now ε instead of $\hbar$. This parameter is introduced to comply with the semiclassical analysis we are about to start. For now, we just consider ε formally as a small parameter. We now only consider classical symbols with asymptotic series in ε, i.e., symbols $A_\varepsilon \in \mathrm{S}^{0,\mathrm{Cl}}_m$ such that

$$A_\varepsilon \asymp \sum_{i \in \mathbb{N}_0} \varepsilon^i A_i. \tag{5.27}$$

Definition 5.1. A symbol $A_\varepsilon \in \mathrm{S}^{0,\mathrm{Cl}}_m\big(\mathrm{T}^*\mathbb{R}^d, \mathscr{B}(\mathscr{H}_0)\big)$ is $\tau-$equivariant (more precisely $(\tau_1, \tau_2)-$equivariant), if

$$A_\varepsilon(r, k-\gamma^*) = \tau_2 A_\varepsilon(r, k)\tau_1^{-1}, \quad \forall \gamma^* \in \Gamma^*. \tag{5.28}$$

The space of $\tau-$equivariant symbols is denoted $\mathrm{S}^\tau_m\big(\mathrm{T}^*\mathbb{T}^d, \mathscr{B}(\mathscr{H}_0)\big)$.

Recall that τ is a unitary representation of the lattice translations on $\mathscr{H}_0$. With this definition, all properties enumerated in section 4.1 are valid for operators $\mathrm{Op}^{\mathrm{w}}_\varepsilon[A]$ with symbols $A \in \mathrm{S}^\tau_m\big(\mathrm{T}^*\mathbb{T}^d, \mathscr{B}(\mathscr{H}_0)\big)$ acting on

$$\mathscr{H}'_\tau = \{\psi(r, k) \in \mathrm{L}^2\big(\mathbb{T}^d, \mathscr{B}(\mathscr{H}_0)\big) : \psi(k-\gamma^*) = \tau(\gamma^*)\psi(k)\}. \tag{5.29}$$

For a complete account see [PST03].

5.2 Perturbed periodic Schrödinger operators

We consider now perturbations of periodic Schrödinger operators. This topic also has a long history, in particular due to the fact that the effective dynamics proposed by Peierls has eluded strict considerations. Peierls stipulated that one would effectively describe the dynamics of perturbed periodic Schrödinger operators by substituting the periodic part of the Hamiltonian by the corresponding band function $\mathscr{E}_n(k)$. In particular, this means that the evolution of a periodic Schrödinger operator with magnetic and electric potentials $\mathscr{A}$ and φ, respectively,

$$\widehat{H}_{\mathrm{EM}} = \frac{\big(-\mathrm{i}\nabla_x - \mathscr{A}(x)\big)}{2} + V_\Gamma(x) + \varphi(x), \tag{5.30}$$

would be approximated by the classical motion generated by

$$h_{\mathrm{Peierls}}(k, r) = \mathscr{E}_n(k - \mathscr{A}(r)) + \varphi(r). \tag{5.31}$$

For Hamiltonians with magnetic potentials, this has only been shown rather recently. Our aim is to introduce multi–scale analysis to study this kind of problems with an emphasis on spectral properties.

5.2.1 Multi–scale approach

The multi–scale approach is an ansatz used to study the properties of systems with distinct scales [GRT88, GMS91, PST03]. The idea is to use these different scales to effectively describe the properties of such systems. In principal, we

start with a full quantum mechanical description and treat the slowly varying degrees of freedom semiclassically.

For our purposes, the perturbations to the periodic potential will act on a much larger scale than the lattice spacing. This can advantageously be written by the perturbation of a magnetic and electric potential of the form $\mathscr{A}(\varepsilon x)$ and $\varphi(\varepsilon x)$ respectively. Treating this asymptotically as $\varepsilon \to 0$ allows us to study the problem in the limit of small perturbations. We can then see the perturbed periodic Schrödinger operator as the $\varepsilon-$Weyl quantization of an operator valued symbol.

Note that the semiclassical treatment is now in ε. It is for that reason that we have set $\hbar = 1$.

We aim to study the properties of the operator

$$\widehat{H}^{\varepsilon} = \frac{\left(-\mathrm{i}\nabla_x - \mathscr{A}(\varepsilon x)\right)^2}{2} + V_\Gamma(x) + \varphi(\varepsilon x). \tag{5.32}$$

The key point here is that $1/\varepsilon$ should be much larger than the period of Γ. We will assume that the Bloch transform[2] of $\widehat{H}^{\varepsilon}$, $\widehat{H}^{\varepsilon}_{\mathrm{BF}} : \mathscr{H}_\tau \to \mathscr{H}_\tau$,

$$\widehat{H}^{\varepsilon}_{\mathrm{BF}} = \frac{\left(-\mathrm{i}\nabla_y + k - \mathscr{A}\left(\mathrm{i}\varepsilon\nabla_k\right)\right)^2}{2} + V_\Gamma(y) + \varphi\left(\mathrm{i}\varepsilon\nabla_k\right), \tag{5.33}$$

is the $\varepsilon-$Weyl quantization of the symbol

$$\widehat{h}^{\varepsilon}_{\mathrm{BF}}(r,k) = \frac{\left(-\mathrm{i}\nabla_y + k - \mathscr{A}(r)\right)^2}{2} + V_\Gamma(y) + \varphi(r). \tag{5.34}$$

In other words, $\mathrm{Op}^{\mathrm{w}}_{\varepsilon}\left[\widehat{h}^{\varepsilon}_{\mathrm{BF}}\right] = \widehat{H}^{\varepsilon}_{\mathrm{BF}}$. We wish to stress that for fixed values of (r,k), $\widehat{h}^{\varepsilon}_{\mathrm{BF}}$ is an operator acting on $\mathrm{L}^2(\mathscr{M})$. The eigenvalue problem for $\widehat{h}^{\varepsilon}_{\mathrm{BF}}$ is nothing else than

$$\left(\frac{\left(-\mathrm{i}\nabla_y + k - \mathscr{A}(r)\right)^2}{2} + V_\Gamma(y) + (\varphi(r) - E)\right)\psi = 0. \tag{5.35}$$

But

$$\widehat{h}_{\mathrm{BF}}(r,k) = \frac{\left(-\mathrm{i}\nabla_y + k - \mathscr{A}(r)\right)^2}{2} + V_\Gamma(y) \tag{5.36}$$

[2]To simplify the notation, the suffices per and τ in ∇_y^{per} and ∇_k^{τ} will be considered implicitly.

has eigenvalues $\mathscr{E}_n(k)$. Hence we have

$$E = \mathscr{E}_n(k - \mathscr{A}(r)) + \varphi(r). \tag{5.37}$$

For fixed (r, k), $\widehat{h}^{\varepsilon}_{\mathrm{BF}}(r, k)$ is an operator on $\mathrm{L}^2(\mathscr{M})$. To an eigenvalue E, we can subscribe the eigenfunction

$$\psi^{\varepsilon}_n(E, k, y) = \psi_n(E - \varphi(r), k, y) \tag{5.38}$$

in $\mathrm{L}^2(\mathscr{M})$ and a spectral projector $\widehat{\pi}_0(r, k) \in \mathscr{B}\left(\mathrm{L}^2(\mathscr{M})\right)$.

5.2.2 The almost projector

Under certain assumptions it is, modulo errors of the order $\mathscr{O}(\varepsilon^\infty)$, possible to construct a projector corresponding to an eigenvalue of the quantization of an operator valued symbol [EW96]. In particular, the principal symbol of this projector will be the spectral projector of the operator valued symbol. We review here a construction of an almost projector $\mathrm{Op}^{\mathrm{w}}_{\varepsilon}[\widehat{\pi}(k, r)]$ corresponding to an eigenvalue of $\mathrm{Op}^{\mathrm{w}}_{\varepsilon}\left[\widehat{h}(k, r)\right]$ where $\widehat{h}(k, r) \in \mathrm{S}^{\tau}_{m}(\mathrm{T}^*\mathscr{M}^*, \mathscr{B}(\mathscr{H}_0))$ is assumed to have eigenvalues $\mathscr{E}_n(k, r)$ and corresponding projectors

$$\widehat{\pi} \in \mathrm{S}^{\tau}_{m}(\mathrm{T}^*\mathscr{M}^*, \mathscr{B}(\mathscr{H}_0)). \tag{5.39}$$

Its principal symbol will be denoted as $\widehat{\pi}_0$. We treat here periodic Schrödinger operators so it is natural to consider $\mathrm{T}^*\mathscr{M}^*$ with $\tau-$equivariant symbols. The same treatment, e.g. on $\mathrm{T}^*\mathbb{R}^d$, can be applied as long as one has a well defined quantization procedure with a corresponding Moyal product.

We must assume here that no level crossings occur.

Lemma 5.1. *Let $\mathscr{E}(k, r)$ be a non degenerate eigenvalue. Then there exists an almost projection $\mathrm{Op}^{\mathrm{w}}_{\varepsilon}[\widehat{\pi}]$ in the sense that*

$$\mathrm{Op}^{\mathrm{w}}_{\varepsilon}[\widehat{\pi}]^2 = \mathrm{Op}^{\mathrm{w}}_{\varepsilon}[\widehat{\pi}] + \mathscr{O}(\varepsilon^\infty), \quad \mathrm{Op}^{\mathrm{w}}_{\varepsilon}[\widehat{\pi}]^* = \mathrm{Op}^{\mathrm{w}}_{\varepsilon}[\widehat{\pi}] \tag{5.40}$$

such that

$$\left[\mathrm{Op}^{\mathrm{w}}_{\varepsilon}\left[\widehat{h}^{\varepsilon}_{\mathrm{BF}}\right], \mathrm{Op}^{\mathrm{w}}_{\varepsilon}[\widehat{\pi}]\right] = \mathscr{O}(\varepsilon^\infty), \tag{5.41}$$

where $\widehat{\pi} \in \mathrm{S}^{\tau}_{m}$ has an asymptotic expansion

$$\widehat{\pi} \asymp \sum_{i \in \mathbb{N}_0} \varepsilon^i \widehat{\pi}_i. \tag{5.42}$$

Its principal symbol $\widehat{\pi}_0(k, r)$ is a spectral projector of $\widehat{h}_{\mathrm{BF}}(r, k)$.

Proof. We follow [EW96]. We proceed iteratively and define

$$\widehat{\pi}_{(k)} = \sum_{i=0}^{k} \varepsilon^i \widehat{\pi}_i. \tag{5.43}$$

We first show that $\widehat{\pi}_{(k+1)}$ is a projection modulo order $\mathcal{O}\left(\varepsilon^{k+1}\right)$. Assuming $\widehat{\pi}_{i\leq k}$ are chosen such that $\widehat{\pi}_{(k)}^2 - \widehat{\pi}_{(k)} = \varepsilon^{k+1}\widehat{r}_k + \mathcal{O}\left(\varepsilon^{k+2}\right)$, we choose $\widehat{\pi}_{k+1}$ such that

$$\widehat{\pi}_0\widehat{\pi}_{k+1} - \widehat{\pi}_{k+1}(1-\widehat{\pi}_0) = \widehat{r}_{k+1}. \tag{5.44}$$

The map

$$\begin{aligned} \mathscr{R} \quad &: \quad \mathrm{S}^{\tau}_{m}(\mathrm{T}^*\mathscr{M}^*, \mathscr{B}(\mathscr{H}_0)) \to \mathrm{S}^{\tau}_{m}(\mathrm{T}^*\mathscr{M}^*, \mathscr{B}(\mathscr{H}_0)) && (5.45)\\ &\widehat{a} \mapsto \widehat{\pi}_0\widehat{a} - \widehat{a}(1-\widehat{\pi}_0), && (5.46) \end{aligned}$$

where $\widehat{\pi}_0\widehat{a} + \widehat{a}(1-\widehat{\pi}_0)$ can be identified with $\widehat{\pi}_0\widehat{a}\widehat{\pi}_0 + (1-\widehat{\pi}_0)\widehat{a}(1-\widehat{\pi}_0)$ for operators that commute with $\widehat{\pi}_0$. By construction the image of this map satisfies $[\widehat{\pi}_0, \mathscr{R}(\widehat{a})]_{\sharp,\varepsilon} = 0$, $\forall \widehat{a} \in \mathscr{B}(\mathscr{H}_0)$.

Thus, by induction such a construction produces a formal symbol that commutes with $\widehat{\pi}_0$ to all orders in ε and is in $\mathrm{S}^{\tau}_{m}(\mathrm{T}^*\mathscr{M}^*, \mathscr{B}(\mathscr{H}_0))$.

Assume now that we have $\widehat{\pi}_{(k)} \in \mathrm{S}^{\tau}_{m}(\mathrm{T}^*\mathscr{M}^*, \mathscr{B}(\mathscr{H}_0))$ with principal symbol $\widehat{\pi}_0$ such that

$$\left[\widehat{h}, \widehat{\pi}_{(k)}\right]_{\sharp,\varepsilon} = \mathcal{O}\left(\varepsilon^{k+1}\right). \tag{5.47}$$

Then there exists a unique $\widehat{f}$ such that

$$\left[\widehat{h}, \widehat{\pi}_{(k)}\right]_{\sharp,\varepsilon} = \varepsilon^{k+1}\widehat{f} + \mathcal{O}\left(\varepsilon^{k+2}\right). \tag{5.48}$$

We write the projector

$$\widehat{\pi}_{(k+1)} = \mathrm{e}^{\varepsilon^{k+1}\widehat{a}}\widehat{\pi}_{(k)}\mathrm{e}^{-\varepsilon^{k+1}\widehat{a}}, \widehat{a} \in \mathrm{S}^{\tau}_{m}(\mathrm{T}^*\mathscr{M}^*, \mathscr{B}(\mathscr{H}_0)), \tag{5.49}$$

which to first order in the exponentials can be written

$$\widehat{\pi}_{(k+1)} = \widehat{\pi}_{(k)} + \varepsilon^{k+1}\left[\widehat{h}, \widehat{a}\right]_{\sharp,\varepsilon} + \mathcal{O}\left(\varepsilon^{k+2}\right). \tag{5.50}$$

Since

$$\left[\widehat{h}, \widehat{\pi}_{(k+1)}\right]_{\sharp,\varepsilon} = \left[\widehat{h}, \widehat{\pi}_{(k)}\right]_{\sharp,\varepsilon} + \varepsilon^{k+1}\left[\widehat{h}, [\widehat{\pi}_0, \widehat{a}]_{\sharp,\varepsilon}\right]_{\sharp,\varepsilon} + \mathcal{O}\left(\varepsilon^{k+2}\right), \tag{5.51}$$

$\widehat{f} \in \mathrm{S}^{\tau}_{m}(\mathrm{T}^{*}\mathscr{M}^{*}, \mathscr{B}(\mathscr{H}_0))$ will fulfill (5.48) by choosing $\widehat{a}$ such that

$$\widehat{f} + \left[\widehat{h}_0, [\widehat{\pi}_0, \widehat{a}]\right] = 0. \tag{5.52}$$

This can be achieved only if $\widehat{\pi}_0 \widehat{f} \widehat{\pi}_0$ and $(1-\widehat{\pi}_0)\widehat{f}(1-\widehat{\pi}_0)$ vanish in leading order of ε. With this choice, we see that

$$\widehat{\pi}_{(k)} \sharp_\varepsilon \left[\widehat{\pi}_{(k)}, \widehat{h}\right]_{\sharp,\varepsilon} \sharp_\varepsilon \widehat{\pi}_{(k)} \tag{5.53}$$

and

$$\left(1-\widehat{\pi}_{(k)}\right) \sharp_\varepsilon \left[1-\widehat{\pi}_{(k)}, \widehat{h}\right]_{\sharp,\varepsilon} \sharp_\varepsilon \left(1-\widehat{\pi}_{(k)}\right) \tag{5.54}$$

also vanish since $\widehat{\pi}_{(k)}$ is a projection. By construction, $\widehat{\pi}$ is unique and

$$\left[\widehat{\pi}, \widehat{h}\right]_{\sharp,\varepsilon} = \mathscr{O}(\varepsilon^{\infty}). \tag{5.55}$$

Hence

$$\left[\mathrm{Op}^{\mathrm{w}}_{\varepsilon}[\widehat{\pi}], \mathrm{Op}^{\mathrm{w}}_{\varepsilon}\left[\widehat{h}\right]\right] = \mathscr{O}(\varepsilon^{\infty}). \tag{5.56}$$

□

As in [PST03] we can introduce a true projector

$$\widehat{\Pi}^{\varepsilon} = \frac{\mathrm{i}}{2\pi} \int_{|\zeta-1|=\frac{1}{2}} \left(\mathrm{Op}^{\mathrm{w}}_{\varepsilon}[\widehat{\pi}] - \zeta\right)^{-1} \mathrm{d}\zeta \tag{5.57}$$

in the sense that it satisfies $\left(\widehat{\Pi}^{\varepsilon}\right)^2 = \widehat{\Pi}^{\varepsilon}$, $\left(\widehat{\Pi}^{\varepsilon}\right)^{*} = \widehat{\Pi}^{\varepsilon}$, $\widehat{\Pi}^{\varepsilon} = \widehat{\pi} + \mathscr{O}(\varepsilon^{\infty})$ and

$$\left\| \left[\widehat{H}^{\varepsilon}_{\mathrm{BF}}, \widehat{\Pi}^{\varepsilon}\right] \right\|_{\mathscr{B}(\mathscr{H}_\tau)} \leq C \left\| \left[\widehat{H}^{\varepsilon}_{\mathrm{BF}}, \widehat{\pi}\right] \right\|_{\mathscr{B}(\mathscr{H}_\tau)} = \mathscr{O}(\varepsilon^{\infty}), \tag{5.58}$$

(see [NS04]).

5.3 Spectral asymptotics

5.3.1 Construction of WKB quasi-modes

We now have the tools to construct a WKB approximation corresponding to the classical motion described by an eigenvalue λ and corresponding classical trajectory $\Lambda(E) \subset \lambda^{-1}(E)$. Note that, when comparing to the previously introduced scalar WKB, the amplitudes will now be vector valued of size N where N is the

dimension of the subspace spanned by $\widehat{\pi}$. The procedure is, under the right assumptions, in essence the same as for the scalar WKB case. Due to the fact that the problem is no longer a scalar one, some additional geometric terms will appear. This section is dedicated to these terms. Such construction can be found in [EW96, LF91] (also see references therein). We restrict here the discussion to $\tau-$equivariant symbols.

The assumptions will, however, be stronger than in the scalar case:

1. $\widehat{h} \in \mathrm{S}^{\tau}_{m}(\mathrm{T}^{*}\mathscr{M}^{*}, \mathscr{B}(\mathscr{H}_0))$ has an asymptotic expansion $\widehat{h} \asymp \sum_{i\in\mathbb{N}_0} \varepsilon^{i}\widehat{h}_i$. $\widehat{h}$ and $\widehat{h}_i$ act on the Hilbert space $\mathscr{H}_0$.

2. For fixed $X \in \mathrm{T}^{*}\mathscr{M}^{*}$, $\widehat{h}_0(X)$ has regular eigenvalues $\lambda(X)$ (of constant multiplicity) with a corresponding smooth projection $\widehat{\pi}_0(X)$. $\psi_\lambda(X)$ is an eigenvector corresponding to $\lambda(X)$.

3. $\widehat{\pi}(X)\mathscr{H}_0$ is the fiber of the $\lambda-$eigenbundle over $\Lambda(E)$.

Once again, we will only consider the one dimensional case for simplicity of notation, i.e., $\dim(\mathscr{M}^{*}) = 1$. The description extend to the multidimensional case similarly as in the scalar WKB case.

We make the usual ansatz

$$\psi_{\mathrm{WKB}} = a_\varepsilon \mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\mathscr{S}(k)}, \quad a_\varepsilon = \sum_{i\in\mathbb{N}_0} \varepsilon^{i} a_i, \tag{5.59}$$

where a_ε will now be vector valued. We note here that the underlying classical system has a phase space $\mathrm{T}^{*}\mathscr{M}^{*}$. The WKB ansatz we have written here is hence in "position" representation. In the spirit of the introduction to the Maslov construction of section 4.7 we will construct quasi–modes locally. Each such local representation will have a corresponding Maslov index. The Maslov index after one revolution on the classical trajectory will be μ. We will here suppress the Maslov phase momentarily since it will only play a role when the corresponding WKB ansatz has to be considered globally. The idea is to use the constructed projection to produce ε^2-quasi–modes.

We seek WKB solutions to

$$\left(\mathrm{Op}^{\mathrm{w}}_{\varepsilon}\left[\widehat{h}\right] - E\right)\psi_{\mathrm{WKB}} = \mathscr{O}\left(\varepsilon^2\right) \tag{5.60}$$

with ψ_{WKB} in the $\lambda-$eigenbundle. We rewrite this equivalently as

$$\mathrm{Op}^{\mathrm{w}}_{\varepsilon}\left[\widehat{\pi}\sharp_\varepsilon\left(\widehat{h} - E\right)\sharp_\varepsilon\widehat{\pi}\right]\psi_{\mathrm{WKB}} = \mathscr{O}\left(\varepsilon^2\right). \tag{5.61}$$

In a first step we calculate the principal and subprincipal symbols of

$$\mathrm{Op}^{\mathrm{w}}_{\varepsilon}\left[\widehat{\pi}\sharp_{\varepsilon}\left(\widehat{h}-E\right)\sharp_{\varepsilon}\widehat{\pi}\right]. \tag{5.62}$$

We then calculate the action of its quantization on a carefully chosen ψ_{WKB} up to order $\mathcal{O}\left(\varepsilon^2\right)$.

In its expansion in ε, the ε^0 terms of $\widehat{\pi}\sharp_{\varepsilon}\left(\widehat{h}-E\right)\sharp_{\varepsilon}\widehat{\pi}$ is nothing else but

$$\widehat{\pi}_0\left(\widehat{h}_0-\lambda\right)\widehat{\pi}_0. \tag{5.63}$$

The next term in the expansion can be calculated using the definition of the Moyal product to

$$\begin{aligned}\mathrm{symb}^{\mathrm{w}}_{\varepsilon,1}\left[\widehat{\pi}\sharp_{\varepsilon}\left(\widehat{h}-\lambda\right)\sharp_{\varepsilon}\widehat{\pi}\right]+\mathrm{symb}^{\mathrm{w}}_{\varepsilon,1}\left[\widehat{\pi}\sharp_{\varepsilon}(\lambda-E)\sharp_{\varepsilon}\widehat{\pi}\right] \;=\; & \\ \widehat{\pi}_0\widehat{h}_1\widehat{\pi}_0+\widehat{\pi}_1\left(\widehat{h}_0-\lambda\right)\widehat{\pi}_0+\widehat{\pi}_0\left(\widehat{h}_0-\lambda\right)\widehat{\pi}_1+ & \\ \frac{\mathrm{i}}{2}\left(\{\widehat{\pi}_0,\left(\widehat{h}_0-\lambda\right)\}\widehat{\pi}_0+\{\widehat{\pi}_0\left(\widehat{h}_0-\lambda\right),\widehat{\pi}_0\}\right)+ & \\ \mathrm{symb}^{\mathrm{w}}_{\varepsilon,1}\left[\widehat{\pi}\sharp_{\varepsilon}(\lambda-E)\sharp_{\varepsilon}\widehat{\pi}\right], &\end{aligned} \tag{5.64}$$

where the notation $\mathrm{symb}^{\mathrm{w}}_{\varepsilon,1}[\cdot]$ has been abused to denote the corresponding term in ε in the expansion. Note that $\widehat{\pi}_0\left(\widehat{h}_0-\lambda\right)$ and $\left(\widehat{h}_0-\lambda\right)\widehat{\pi}_0$ vanish when a_{ε} is in the $\lambda-$eigenbundle. Hence only

$$\widehat{\pi}_0\widehat{h}_1\widehat{\pi}_0+\frac{\mathrm{i}}{2}\widehat{\pi}_0\{\widehat{\pi}_0,\left(\widehat{h}_0-\lambda\right)\}\widehat{\pi}_0+\mathrm{symb}^{\mathrm{w}}_{\varepsilon,1}\left[\widehat{\pi}\sharp_{\varepsilon}(\lambda-E)\sharp_{\varepsilon}\widehat{\pi}\right] \tag{5.65}$$

remain in that case. In view of (5.61), if E is an eigenvalue of $\widehat{h}$, by assumption, $\lambda-E$ is of order $\mathcal{O}(\varepsilon)$ since λ is an eigenvalue of the principal symbol of $\widehat{h}$. Hence, again expanding the Moyal product up to order $\mathcal{O}(\varepsilon)$

$$\begin{aligned}\mathrm{symb}^{\mathrm{w}}_{\varepsilon,1}\left[\widehat{\pi}\sharp_{\varepsilon}(\lambda-E)\sharp_{\varepsilon}\widehat{\pi}\right] &= \mathrm{symb}^{\mathrm{w}}_{\varepsilon,1}\left[\widehat{\pi}_0\sharp_{\varepsilon}(\lambda-E)\sharp_{\varepsilon}\widehat{\pi}_0\right] &(5.66)\\ &= \frac{\mathrm{i}}{2}(\{\widehat{\pi}_0,\lambda\}\widehat{\pi}_0+\widehat{\pi}_0\{\lambda,\widehat{\pi}_0\}). &(5.67)\end{aligned}$$

Formally, we can rewrite $\{\widehat{\pi}_0,\lambda\}$ as

$$\{\widehat{\pi}_0^2,\lambda\}=\{\widehat{\pi}_0,\lambda\}\widehat{\pi}_0+\widehat{\pi}_0\{\widehat{\pi}_0,\lambda\} \tag{5.68}$$

since $\widehat{\pi}_0$ is a projector. We intend to calculate (5.66) which is an expression with $\widehat{\pi}_0$ to the right and to the left. With this in mind we may always add a $\widehat{\pi}_0$ to the right and the left of the expressions in (5.67) since $\widehat{\pi}_0 = \widehat{\pi}_0^2$. We may then write

$$\begin{aligned} \widehat{\pi}_0\{\widehat{\pi}_0, \lambda\}\widehat{\pi}_0 &= \widehat{\pi}_0\{\widehat{\pi}_0^2, \lambda\}\widehat{\pi}_0 && (5.69)\\ &= \widehat{\pi}_0\{\widehat{\pi}_0, \lambda\}\widehat{\pi}_0 + \widehat{\pi}_0\{\widehat{\pi}_0, \lambda\}\widehat{\pi}_0 && (5.70)\\ &= 2\widehat{\pi}_0\{\widehat{\pi}_0, \lambda\}\widehat{\pi}_0, \end{aligned}$$

which makes sense if and only if $\widehat{\pi}_0\{\widehat{\pi}_0, \lambda\}\widehat{\pi}_0 = -\widehat{\pi}_0\{\lambda, \widehat{\pi}_0\}\widehat{\pi}_0 = 0$. Summum summare, we have

$$\widehat{\pi}\sharp_\varepsilon\left(\widehat{h} - E\right)\sharp_\varepsilon\widehat{\pi} = \widehat{\pi}_0\left(\widehat{h}_0 - \lambda + \varepsilon\left(\widehat{h}_1 + \frac{\mathrm{i}}{2}\{\widehat{\pi}_0, \left(\widehat{h}_0 - \lambda\right)\}\right)\right)\widehat{\pi}_0 + \mathscr{O}\left(\varepsilon^2\right). \quad (5.71)$$

For a function ψ_{WKB} in the image of $\widehat{\pi}$ with energy E, we may write the latter equality

$$\widehat{h}\psi_{\mathrm{WKB}} = \widehat{\pi}_0\left(\lambda\mathbb{1} - \varepsilon\left(\widehat{h}_1 + \frac{\mathrm{i}}{2}\{\widehat{\pi}_0, \left(\widehat{h}_0 - \lambda\right)\}\right)\right)\widehat{\pi}_0\psi_{\mathrm{WKB}} + \mathscr{O}\left(\varepsilon^2\right). \quad (5.72)$$

Using the definition of the Weyl quantization we calculate $\mathrm{Op}_\varepsilon^{\mathrm{w}}\left[\widehat{h}\right]\psi_{\mathrm{WKB}}$ given by the integral (see, e.g. [Vor76])

$$\frac{1}{(2\pi\varepsilon)}\int_{\mathrm{T}^*\mathscr{M}^*}\widehat{h}\left(\frac{k+x}{2}, r\right)a_\varepsilon(x)\mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\mathscr{S}(x)}\mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}(k-x)r}\,\mathrm{d}x\mathrm{d}r. \quad (5.73)$$

Again, for ψ_{WKB} in the range of $\widehat{\pi}$ we get in leading order ε^0

$$\lambda\left(\frac{\partial\mathscr{S}}{\partial k}, k\right)a_0(k), \quad (5.74)$$

which will be equal to Ea_0 if $\mathscr{S}$ is the action corresponding to the motion generated by the Hamiltonian function λ with energy E. The next term is calculated to yield

$$\widehat{\pi}_0\lambda a_1 + \widehat{\pi}_0\frac{\partial\lambda}{\partial r}\frac{\mathrm{d}a_0}{\mathrm{d}k} + \widehat{\pi}_0\frac{1}{2}\frac{\partial^2\lambda}{\partial k\partial r}a_0 + \mathrm{i}\widehat{\pi}_0\left(\widehat{h}_1 + \frac{\mathrm{i}}{2}\{\widehat{\pi}_0, \left(\widehat{h}_0 - \lambda\right)\}\right)\widehat{\pi}_0 a_0 \quad (5.75)$$

where we have suppressed the arguments in $\mathrm{T}^*\mathscr{M}^*$ since all terms should be associated to $\Lambda(E)$. Now setting $a_{i\geq 1} = 0$, we must demand that

$$\widehat{\pi}_0\frac{\partial\lambda}{\partial r}\frac{\mathrm{d}a_0}{\mathrm{d}k} + \widehat{\pi}_0\frac{1}{2}\frac{\partial^2\lambda}{\partial k\partial r}a_0 - \mathrm{i}\widehat{\pi}_0\left(\widehat{h}_1 + \frac{\mathrm{i}}{2}\{\widehat{\pi}_0, \left(\widehat{h}_0 - \lambda\right)\}\right)\widehat{\pi}_0 a_0. \quad (5.76)$$

The two first terms are recognized from the scalar WKB. We therefore rewrite the ansatz as $a_0 = u\nu$ where ν is a scalar and $u \in \mathbb{C}^N \otimes \mathscr{H}_0$ is in the image of $\widehat{\pi}$. Insertion gives now

$$\widehat{\pi}_0 \frac{\partial \lambda}{\partial r}\frac{\mathrm{d}u}{\mathrm{d}k} - \mathrm{i}\widehat{\pi}_0\left(\widehat{h}_1 - \frac{1}{2}\left(\widehat{\pi}_0\{\widehat{\pi}_0, \left(\widehat{h}_0 - \lambda\right)\}\right)\right)\widehat{\pi}_0 u \tag{5.77}$$

and as expected from the scalar WKB

$$\nu = \left(\left|\frac{\partial \mathscr{S}}{\partial k}\right|\right)^{-\frac{1}{2}}. \tag{5.78}$$

With this ψ_{WKB} is a quasi–mode if the latter vanishes, i.e., we find a transport equation

$$\widehat{\pi}_0 \frac{\mathrm{d}u}{\mathrm{d}t} - \mathrm{i}\widehat{\pi}_0\left(\widehat{h}_1 - \frac{1}{2}\{\widehat{\pi}_0, \left(\widehat{h}_0 - \lambda\right)\}\right)\widehat{\pi}_0 u = 0, \tag{5.79}$$

where we have re–parametrized $\Lambda(E)$ with t since, using Hamilton's equation of motion $\frac{\partial \lambda}{\partial r} = \dot{k}$, so

$$\frac{\partial \lambda}{\partial r}\frac{\mathrm{d}u}{\mathrm{d}k} = \dot{k}\frac{\partial u}{\partial k} = \frac{\mathrm{d}u}{\mathrm{d}t}.$$

Such terms are discussed in [EW96] and can be interpreted in terms of geometrical objects[3]. We can see $u(t) = U(t)v$ as a smooth section in the $\lambda-$eigenbundle over $\Lambda(E)$ with $u(0) = v$ and $U(t) \in \mathrm{U}(N)$. In other words, U is a $\lambda-$eigenbundle endomorphism which can be seen as the holonomy of a parallel transport. More specifically, choosing a normalized section in the $\lambda-$eigenbundle, represented by

$$\psi_\lambda = \left(\psi_{\lambda,1}, \psi_{\lambda,2}, ..., \psi_{\lambda,N}\right), \tag{5.80}$$

the projector may be written $\widehat{\pi}_0 = \psi_\lambda \psi_\lambda^*$ whereupon (5.79) takes the form in [LF91],

$$\frac{\mathrm{d}u}{\mathrm{d}t} = \mathrm{i}\sum_{i=1}^{N}\left[\psi_{\lambda,i}\{\psi_{\lambda,i}, \lambda\} + \sum_{j=i}^{N}\widehat{h}_{0,i,j}\{\psi_{\lambda,i}, \psi_{\lambda,j}\}\right] u \tag{5.81}$$

$$-\psi_\lambda \psi_\lambda^* \widehat{h}_1 \psi_\lambda \psi_\lambda^* u, \tag{5.82}$$

where $\widehat{h}_{0,i,j}$ are the matrix elements of $\widehat{h}_0$. Such results originate in the calculations of [BL83] and were put in the above form using Poisson brackets by

[3] An introduction to differential geometry can be found in [Bre97, NS87, Nak03].

[KYH87]. The first term will be called Berry term and the second curvature term according to the nomenclature in [EW96]. The name Berry term comes from the fact that it can be interpreted as the holonomy of a projected connection. Such holonomies result in phase factors identified as Berry phases by B. Simon [Sim83] as a remark on a phase introduced by M. Berry [Ber84].

For further reference, we note that in the case of a non–degenerate eigenvalue, the fiber is $\mathbb{C}^1$ and the action of the holonomy is merely U(1) with values

$$\tau(\Lambda(E)) = \mathrm{e}^{\mathrm{i}(\gamma_{\mathrm{B}}+\gamma_{\mathscr{C}}+\gamma_1)}. \tag{5.83}$$

The Berry term contributes with

$$\gamma_{\mathrm{B}} = \int_{\Lambda(E)} \psi_\lambda^* \,\mathrm{d}\psi_\lambda \tag{5.84}$$

and the curvature term

$$\gamma_{\mathscr{C}} = \int_{\Lambda(E)} \widehat{h}_0\{\psi_\lambda, \psi_\lambda^*\}, \tag{5.85}$$

will not contribute since $\{\psi_\lambda, \psi_\lambda^*\} = 0$. The last term

$$\gamma_1 = \int_{\Lambda(E)} \psi_\lambda \psi_\lambda^* \widehat{h}_1 \psi_\lambda \psi_\lambda^* \tag{5.86}$$

originates in the subprincipal symbol $\widehat{h}_1$ of $\widehat{h}$. With this, our ansatz takes the form

$$\psi_{\mathrm{WKB}}(k) = \mathrm{e}^{\mathrm{i}\left(\frac{\mathscr{S}(k)}{\varepsilon} - \frac{\pi}{4}\mu + \gamma_{\mathrm{B}}(k) + \gamma_1(k)\right)} \nu(k)\psi_\lambda(k) + \mathscr{O}\left(\varepsilon^2\right), \tag{5.87}$$

where $\nu(k)$ is given by (5.78). The ansatz is here written on a chart parametrized by $k \to \left(\frac{\partial \mathscr{S}}{\partial k}, k\right)$ where we have included the corresponding Maslov index μ.

Notice that, (5.79) is nothing else than a first order periodic ODE, since the transport is along a loop. Hence, the flow generated by λ is periodic along that loop, $\widehat{\pi}_0(k)$, $\widehat{h}_0(k)$, $\widehat{h}_1(k)$ will be also be periodic. One expects, hence, u to have a Floquet solution

$$u(k) = \mathrm{e}^{\mathrm{i}Kk} P(k), \quad P(k) = P(k + L_E) \tag{5.88}$$

where L_E is the length of the corresponding trajectory and K the corresponding Floquet matrix. So we could also see the holonomy around $\Lambda(E)$ as a Floquet multiplier matrix.

5.3.2 Quantization of perturbed periodic systems

Now, we assume $\widehat{h}$ above to have the form

$$\widehat{h} \asymp \sum_{i \in \mathbb{N}_0} \varepsilon^i \widehat{h}_i, \quad \widehat{h}_1 = 0 \tag{5.89}$$

where

$$\widehat{h}_i \in \mathrm{S}^{\tau}_{p}\left(\mathrm{T}^*\mathscr{M}^*, \mathscr{B}\left(\mathrm{L}^2(\mathscr{M})\right)\right). \tag{5.90}$$

In other words, we consider only $\tau-$equivariant symbols whose subprincipal symbol vanishes such as $\widehat{H}^{\varepsilon}_{\mathrm{BF}}$ (section 5.2.1). As discussed above, we assume $\widehat{h}_0 = \widehat{h}^{\varepsilon}_{\mathrm{BF}}$ (again, see section 5.2.1) has smooth eigenvalues on $\mathrm{T}^*\mathscr{M}^*$ (this is at least true for $d \leq 3$ see [Pan07]). In particular we consider the mth eigenvalue of the principal symbol of $\widehat{h}$

$$\lambda(r, k) = \mathscr{E}_m(k - \mathscr{A}(r)) + \varphi(r), \tag{5.91}$$

which will be assumed to have constant multiplicity one (this is always satisfied in one dimension, see Theorem 5.1).

According to the previous section, we can construct ε^2-quasi-modes of the form (see (5.87))

$$\psi_{\mathrm{WKB}}(k, y) = \mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\mathscr{S}(k) + \mathrm{i}\left(\gamma_{\mathrm{B}}(k) - \frac{\pi}{4}\mu\right)} \nu(k) \psi^{\varepsilon}_m(k, y) \tag{5.92}$$

corresponding to an energy E and $\mathrm{e}^{\mathrm{i}\gamma_{\mathrm{B}}(k)} \in \mathrm{U}(1)$ is given by the holonomy described above. Since the multiplicity of the eigenvalue is one, the curvature term $\gamma_{\mathscr{C}}$ in (5.83) vanishes. The action will be associated to the classical trajectory $\Lambda(E)$ described by $\lambda(r, k)$. The reduced action corresponding to the motion is given by

$$\mathscr{S}(k) = \int_{k_0}^{k} r \, \mathrm{d}x, \tag{5.93}$$

along the trajectory $\Lambda(E)$.

Note that by assumption the subprincipal symbol of $\widehat{h}$ is zero, hence, we have $\gamma_1 = 0$.

In order for $\psi_{\mathrm{WKB}}(k, y)$ to be a quasi-mode, it must be an element of $\mathscr{H}_{\tau}$, i.e.,

$$\psi_{\mathrm{WKB}}(k - \gamma^*, y) = \mathrm{e}^{\mathrm{i}\gamma^* y} \psi_{\mathrm{WKB}}(k, y), \forall \gamma^* \in \Gamma^*, \tag{5.94}$$

$$\psi_{\mathrm{WKB}}(k, y + \gamma) = \psi_{\mathrm{WKB}}(k, y), \forall \gamma \in \Gamma. \tag{5.95}$$

If we were constructing an ε^∞ quasi–mode, we would have to demand that this be satisfied to all orders in ε. Since we merely seek for ε^2 quasi–modes, it suffices to demand that (5.94) and (5.95) be satisfied to $\mathcal{O}\left(\varepsilon^2\right)$. Since we also must consider the Maslov correction (see section 4.7) we denote μ the corresponding Maslov index.

Furthermore, the action $\mathscr{S}(k \pm \gamma^*)$ along the classical trajectory is,

$$\begin{aligned} \mathscr{S}(k \pm \gamma^*) &= \int_{k_0}^{k \pm \gamma^*} r \, \mathrm{d}x && (5.96) \\ &= \int_{k_0}^{k} r \, \mathrm{d}x \pm \oint_{\Lambda(E)} r \, \mathrm{d}x && (5.97) \\ &= \mathscr{S}(k) \pm \mathscr{S}(\gamma^*). && (5.98) \end{aligned}$$

It is readily seen that the Berry term γ_{B} has the same property. Now, we have to demand that (5.94) is satisfied. We have

$$\psi_{\mathrm{WKB}}(k-\gamma^*, y) = \mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\mathscr{S}(k-\gamma^*)+\mathrm{i}\left(\gamma_{\mathrm{B}}(k-\gamma^*)-\frac{\pi}{4}\mu\right)} \nu(k-\gamma^*) \psi_m^\varepsilon(k-\gamma^*, y), \qquad (5.99)$$

where we have taken into account the Maslov index μ along one revolution of $\Lambda(E)$ (in the direction opposite to the classical motion induced by λ). Since $\psi_m^\varepsilon(k, y)$ is in $\mathscr{H}_\tau$, we have

$$\psi_m^\varepsilon(k-\gamma^*, y) = \mathrm{e}^{\mathrm{i}\gamma^* y} \psi_m^\varepsilon(k, y), \qquad (5.100)$$

hence

$$\psi_{\mathrm{WKB}}(k-\gamma^*, y) = \mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\mathscr{S}(k-\gamma^*)+\mathrm{i}\left(\gamma_{\mathrm{B}}(k-\gamma^*)-\frac{\pi}{4}\mu\right)} \nu(k-\gamma^*) \mathrm{e}^{\mathrm{i}\gamma^* y} \psi_m^\varepsilon(k, y). \qquad (5.101)$$

Now, using the above property of the action and Berry term we can write

$$\mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\mathscr{S}(k-\gamma^*)+\mathrm{i}\left(\gamma_{\mathrm{B}}(-\gamma^*)-\frac{\pi}{4}\mu\right)} = \mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\mathscr{S}(k)+\mathrm{i}\gamma_{\mathrm{B}}(k)} \mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}\mathscr{S}(\gamma^*)+\mathrm{i}\left(-\gamma_{\mathrm{B}}(\gamma^*)-\frac{\pi}{4}\mu\right)}. \qquad (5.102)$$

The fact that ν is k–periodic, implies

$$\begin{aligned} \psi_{\mathrm{WKB}}(k-\gamma^*, y) &= \mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\mathscr{S}(k)+\mathrm{i}\gamma_{\mathrm{B}}(k)} \mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\mathscr{S}(-\gamma^*)+\mathrm{i}\left(\gamma_{\mathrm{B}}(-\gamma^*)-\frac{\pi}{4}\mu\right)} \nu(k) \mathrm{e}^{\mathrm{i}\gamma^* y} \psi_m^\varepsilon(k, y) \\ &= \mathrm{e}^{\mathrm{i}\gamma^* y} \psi_{\mathrm{WKB}}(k, y) \left(\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}\mathscr{S}(\gamma^*)+\mathrm{i}\left(-\gamma_{\mathrm{B}}(\gamma^*)-\frac{\pi}{4}\mu\right)} \right). \end{aligned}$$

According to (5.94), we must therefore demand that the last term in parenthesis is 1, i.e.,

$$\oint_{\Lambda(E)} r \, \mathrm{d}k = 2\pi\varepsilon \left(n + \frac{\mu}{4} - \frac{\gamma_{\mathrm{B}}(\gamma^*)}{2\pi} \right), \, n \in \mathbb{Z}, \qquad (5.103)$$

where the Maslov index μ, as the action and the Berry term, now corresponds to the cycle along $\Lambda(E)$ in the direction of the classical motion given by λ.

The second equation, (5.95), is automatically satisfied,

$$\psi_{\mathrm{WKB}}(k, y+\gamma) = \psi_{\mathrm{WKB}}(k, y), \quad \forall \gamma \in \Gamma, \tag{5.104}$$

by the $y-$periodicity of $\psi^{\varepsilon}_{m}(k, y)$.

We hence get a Bohr–Sommerfeld quantization condition with an additional geometric term expressed by the holonomy of the transport on $\Lambda(E)$ defined by (5.82).

In the physical literature, similar approaches have been proposed to yield such quantization results in the past. Notably, Wilkinson constructed a Bohr–Sommerfeld quantization for Harper's equation that included Berry's phase. This was done by considering a WKB ansatz [Wil84a, Wil84b]. More recently, quantization results have been proposed for more general perturbed periodic Schrödinger operators with electromagnetic potential. The results are derived from effective descriptions of the center of a wave packet [CN95, CN96, SN99] (in essence the classical mechanics given by Peierls' substitution up to corrections). The quantization is a result of demanding that the corresponding action of the effective motion follow an EBK quantization condition. The consideration also incorporates the Berry and Maslov terms in the quantization condition. Results in the strong magnetic field regime are also stated.

For each eigenvalue with number m, this quantization condition defines a family of approximate energies E^{n}_{m} with WKB wave function $\psi_{\mathrm{WKB}}(k)$, an ε^2-quasi–mode by construction. Its Bloch–Floquet inverse is just the Fourier transform to $\mathrm{L}^2(\mathbb{R})$, i.e.,

$$\left(\mathscr{U}^{-1}_{\mathrm{BF}}\psi_{\mathrm{WKB}}\right)(x) = \int_{\mathscr{M}^*} \mathrm{e}^{\mathrm{i}k\cdot x}\psi_{\mathrm{WKB}}(k, [x])\,\mathrm{d}k \tag{5.105}$$

is an ε^2 quasi–mode of $\widehat{H}^{\varepsilon}$.

5.3.3 General states

In the previous section, we have quantized with states the λ–eigenbundle corresponding to a specific energy band. Similarly, one can construct more general states considering the above transport generated by $K < \infty$ such bands with indices in $\mathscr{I}_K$. The fibers will then be equivalent to $\mathbb{C}^K$ and not only $\mathbb{C}^1$ as previously. Again, we must assume that the considered eigenvalues are smooth and have a constant multiplicity one.

The WKB ansatz takes the form

$$\psi_{\mathrm{WKB}}(k,y)=\prod_{i\in\mathscr{I}_K}\psi^i_{\mathrm{WKB}}(k,y), \tag{5.106}$$

where the product ranges over the indices and ψ^i_{WKB} are the above constructed states for one band i. As previously, this potential quasi–mode must be in $\mathscr{H}_\tau$. The different band eigenfunctions are all $\gamma-$periodic and gain a phase factor $\mathrm{e}^{\mathrm{i}\gamma^* y}$ upon a translation of $-\gamma^*$ in k. So, similarly to the one band situation, the resulting quantization condition is reduced to K one dimensional quantization conditions. Note, once again, that we get ε^2-quasi–modes without considering tunneling between the different bands.

5.3.4 A note on degenerate eigenvalues

If we now consider an N fold degenerate energy band, we have to consider the transport along a classical trajectory $\Lambda(E)$ on a fiber $\mathbb{C}^N$ instead of $\mathbb{C}^1$ as we did in the latter examples. In the $\mathbb{C}^1$ case, the EBK quantization procedure was possible since the underlying classical dynamics was integrable and because the holonomy defined by the corresponding transport was U(1).

The quantization procedure we have described above emerges by demanding the single valuedness of the WKB ansatz. In practice, ψ_{WKB} is to $\mathscr{O}\left(\varepsilon^2\right)$ a product of a section ψ_λ in the (smooth) λ–eigenbundle over $\Lambda(E)$, the scalar $\mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\mathscr{S}}/\sqrt{\mathscr{S}'}$ and the holonomy τ along $\Lambda(E)$. Single valuedness of the WKB ansatz results in

$$\mathbb{1}_{N\times N}=\mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\mathscr{S}}\tau(\Lambda(E)) \tag{5.107}$$

since ψ_λ is assumed $\Lambda(E)$–periodic. In order for this condition to make sense, the holonomy τ along $\Lambda(E)$ should be diagonalizable and gauge invariant, i.e., the quantization procedure should be equivalent to N quantizations where τ contributes to each a U(1) phase[4].

We introduce a characterization of an extended version of integrability criteria of Liouville and Arnold [Kep03]. Under these conditions of this characterization, the quantization is reduced to N scalar quantization problems each with a U(1) phase.

We first assume that the classical motion induced by the band function is integrable. The integrability according to the Liouville–Arnold Theorem 3.3 is expressed by the fact that there exist d independent functions A_i satisfying

$$\{A_i,A_j\}=0. \tag{5.108}$$

[4]We refer here to [EW96] who discusses such integrability problems on a more general footing.

Since the energy is constant we set $A_1 = \lambda$.

The integrability condition can be extended in the following way. For this purpose, we define d matrices $\mathfrak{M}_j : \mathrm{T}^*M \to \mathfrak{u}(N)$ that define holonomies τ_j along $\Lambda(E)$ by

$$\frac{\mathrm{d}\tau_j(t)}{\mathrm{d}t} + \mathfrak{M}_j \tau_j(t) = 0 \tag{5.109}$$

where $\mathfrak{u}(N)$ denotes the Lie algebra of $\mathrm{U}(N)$. We also define the extended flow corresponding to the flow Φ^t_λ and the holonomy τ along Φ^t_λ, e.g.,

$$\mathscr{Y}^t_{\lambda,\mathfrak{M}} \quad : \quad \mathrm{T}^*M \times \mathrm{U}(N) \to \mathrm{T}^*M \times \mathrm{U}(N), \tag{5.110}$$

$$(X, g) \mapsto \left(\Phi^t_\lambda(X), \tau(t)g\right). \tag{5.111}$$

In a similar fashion we define the d extended flows $\mathscr{Y}_{A_j,\mathfrak{M}_j}$

$$\mathscr{Y}^t_{A_j,\mathfrak{M}_j} \quad : \quad \mathrm{T}^*M \times \mathrm{U}(N) \to \mathrm{T}^*M \times \mathrm{U}(N) \tag{5.112}$$

$$(X, g) \mapsto \left(\Phi^t_j(X), \tau_j(t)g\right), \tag{5.113}$$

where the flows Φ^t_j are given by the observables $A_j : \mathrm{T}^*M \to \mathbb{R}$ and the holonomies τ_j are given by the transports given by $\mathfrak{M}_j$ along the corresponding flow line of Φ^t_j, i.e., along the cycles $\mathscr{C}_j$ in the language of section 4.8.

The system is deemed integrable if there exists d matrices $\mathfrak{M}_j$,

$$\{A_j, \mathfrak{M}_k\} + \{\mathfrak{M}_j, A_k\} + \left[\mathfrak{M}_j, \mathfrak{M}_k\right] = 0, \tag{5.114}$$

such that $\mathscr{Y}^t_{\lambda,\mathfrak{M}}$ decomposes in d independent extended flows $\mathscr{Y}^t_{A_j,\mathfrak{M}_j}$. In that case, one can show that the group of holonomies along the flow lines of $\Phi^{t_1}_1 \circ \ldots \circ \Phi^{t_d}_d$ is an Abelian subgroup of $\mathrm{U}(N)$.

In analogy to section 4.8, we concentrate on the d cycles $\mathscr{C}_i$. More precisely we consider a WKB ansatz corresponding to the extended flow lines of $\mathscr{Y}^{t_1}_{A_1} \circ \ldots \circ \mathscr{Y}^{t_d}_{A_d}$. As in section 4.8, we construct a corresponding WKB ansatz. From the independence of the extended flows $\mathscr{Y}^t_{A_j,\mathfrak{M}_j}$, we know that the holonomies, τ_i, along different cycles $\mathscr{C}_i$ commute. In such a case, these holonomy matrices have a common basis of eigenvectors. We can hence separate the holonomy matrix along a flow line of $\Phi^{t_1}_1 \circ \ldots \circ \Phi^{t_d}_d$, τ, as the product of d diagonal holonomy matrices each corresponding to a cycle $\mathscr{C}_i$. The holonomy matrix is then similar to the product of the d diagonal holonomies. We can write the action corresponding to a flow line of $\Phi^{t_1}_1 \circ \ldots \circ \Phi^{t_d}_d$ as a sum of action contributions each

from a cycle $\mathscr{C}_i$. At each point along a flow line $\Phi_1^{t_1} \circ ... \circ \Phi_d^{t_d}$, the WKB ansatz will be characterized by a set of d such holonomies and d such actions. Each such pair corresponds to a cycle $\mathscr{C}_i$. If we choose a section in the $\lambda-$eigenbundle such that the holonomy along $\mathscr{C}_i$ is diagonal, we see that it is enough to associate N (U(1)) eigenvalues of the corresponding holonomy and one action to the loop $\mathscr{C}_i$.

Having represented the holonomy diagonally, we need only repeat the arguments of section 4.8 using the d commuting extended flows rather than d commuting flows in order to formulate an EBK quantization. The single valuedness of the WKB ansatz has to be replaced by demanding that (5.107) is satisfied. A consistent solution is obtained if the holonomy around some closed cycle has the form

$$\tau = \mathrm{e}^{\mathrm{i}u} \mathbb{1}_{N\times N}, \quad u \in \mathrm{U}(1). \tag{5.115}$$

More precisely, one can choose a section in the $\lambda-$eigenbundle which corresponds to an eigenvalue of τ along $\mathscr{C}_i$. In such a way, (5.115) is automatically satisfied. One obtains in such a way quantization conditions for each cycle $\mathscr{C}_i$ and each eigenvector of τ. The extension of the flows results in an additional factor that gives a term of order ε in the quantization condition (like the Berry and curvature terms in our case) resulting in the EBK quantization condition analogous to (4.98). One considers the action along a cycle $\mathscr{C}_i$

$$\mathscr{I}_i = \frac{1}{2\pi} \oint_{\mathscr{C}_i} r \, \mathrm{d}k, \tag{5.116}$$

the corresponding Maslov index μ_i (see section 4.8) and $\mathrm{e}^{\mathrm{i}u_r}$ the rth eigenvalue of the holonomy along $\mathscr{C}_i$. The corresponding EBK quantization condition is then

$$\mathscr{I}_i = \varepsilon\left(n + \frac{\mu_i}{4} - \frac{u_r}{2\pi}\right), \quad r = 1, ..., N, \, i = 1, ..., d, \, n \in \mathbb{Z}. \tag{5.117}$$

One example of such degenerate eigenvalues is the case of degenerate spin degrees of freedom which is treated explicitly in [Kep03].

5.4 The Wannier–Stark System

Over the past fifty years, there has been an interest in the Wannier–Stark system. It represents a class of perturbed periodic Schrödinger type operators without magnetic potential. The perturbation is a linear term in position, i.e.,

$$\widehat{H}_{\mathrm{WS}} = -\frac{\Delta_x}{2} + V_\Gamma(x) + \varepsilon x, \tag{5.118}$$

acting on $L^2(\mathbb{R})$. The Wannier–Stark system has long been investigated. This system is relatively simple. It describes effectively a charged particle in a solid under the influence of an electric field, i.e., an experimental realization is feasible. The understanding of such a system is thus conceptually central in the theory of solid state physics. In fact there has been a long standing discussion about the properties of such systems. These discussions were initiated by the counter intuition of the predictions and by a difficulty to verify the predictions experimentally. We will treat here two such properties, namely, Bloch–oscillation[5] and what is commonly called the Wannier–Stark ladder.

Already Bloch [Blo28] and Zener [Zen34] suggested that a localized particle would, under the influence of such a system, exhibit oscillations. In the conventional $\hbar-$semiclassics, one would imagine the particle oscillating in one potential well. The Bloch oscillation is, however, a pure quantum effect and it describes, contrarily to the previous intuition, the periodic motion of a localized particle over several potential wells. The motion of such particles are effectively described by Peierls' substitution. Assuming that the unperturbed spectrum of the periodic operator $-\frac{\triangle}{2} + V_\Gamma(x)$ be given by functions $\mathscr{E}_m(k)$, Peierls' substitution consists in replacing the periodic part of the Hamiltonian by this band function. In leading order, the motion of the center of the localized state would then be given by the motion generated by the classical Hamiltonian $\mathscr{E}_m(k) + \varepsilon q$ where (q, k) are taken as canonical coordinates.

The well foundedness of Peierls' substitution has in itself been the subject of many investigations (we refer here, e.g., to [DGR02, GMS91, Nen90] and references therein). Propagation theorems, e.g., in the form of semiclassical Egorov theorems where the classical Hamiltonian is given by Peierls' substitution, have been proved. We refer here mainly to Panati, Spohn and Teufel who have, amongst others, produced such an Egorov theorem to $\mathscr{O}\left(\varepsilon^2\right)$ for a rather general class of perturbed periodic Schrödinger operators with magnetic potential [PST03]. These considerations include the next order corrections in ε to Peierls' substitution.

The localization properties have also raised quite some interest [HKKM04, WKKM04] as they play an important role, e.g., in the experimental observability of such Bloch oscillations (see e.g., [RS97]). This was particularly interesting since the Bloch–oscillations remained difficult to confirm experimentally. Two effects play an important contribution to this problem. Different energy bands have different dispersions. Hence, inter–band (Zener) tunneling contribute to the dispersion of the particle. Furthermore, the effective dynamics on one band subspace may disperse the particle wave function.

Another, long standing question has been the existence of so–called Wan-

[5] also called Bloch–Zener oscillations.

nier–Stark ladders [Avr76, GKK02, CH91]. These were first described by Wannier as a series of energies in the spectrum of the Wannier–Stark Hamiltonian [Wan60, Wan62, WF62]. To each such energy corresponds a localized state. Note that the results of [CH91] insure that the spectrum of $\widehat{H}_{\mathrm{WS}}$ remains absolutely continuous for fairly general periodic potentials if the perturbation is small enough, i.e., as $\varepsilon \to 0$. The Wannier–Stark ladders are hence better characterized as resonances of $\widehat{H}_{\mathrm{WS}}$ embedded in the absolutely continuous spectrum.

We first address the question of the Wannier–Stark resonances. To our disposal are the tools developed in the earlier sections which we will see produce quasi–energies with corresponding localized quasi–modes. We will use properties of the constructed quasi–energies to describe the evolution of localized states. We consider only a one dimensional system for now. According to Theorem 5.1, no eigenvalue crossings occur in this case except possibly at the extremes of the Brillouin zone. The corresponding eigenfunctions depend smoothly on (r, k). A similar treatment could be carried out for any dimension under such assumptions.

We concentrate first on the resonances of the Wannier–Stark ladder. These resonances will then play a role in the localization of the Bloch oscillations of localized states.

5.4.1 Spectral properties

We consider formally the spectral problem

$$\left(\widehat{H}_{\mathrm{WS}} - E\right)\psi = \mathcal{O}\left(\varepsilon^2\right)$$

where ψ is in the eigenbundle corresponding to the mth energy band of the unperturbed Hamiltonian. This problem is nothing else than an example of the above quantization procedure.

Since we are restrained to one band with index m, the curvature term $\gamma_{\mathscr{C}}$ (5.85) is also zero. Furthermore, $\widehat{H}_{\mathrm{WS}}$ can be seen as the ε–Weyl quantization of

$$\widehat{h}^{\varepsilon}_{\mathrm{BF}}(r, k) = \frac{\left(-\mathrm{i}\nabla_y + k\right)^2}{2} + V_{\Gamma}(y) + r, \tag{5.119}$$

which is ε independent (see section 5.2.1). We hence see that the subprincipal symbol of $\widehat{H}_{\mathrm{WS}}$ is zero which in its turn implies $\gamma_1 = 0$ in (5.87).

The classical dynamics generated by the eigenvalue of the principal symbol of $\widehat{H}_{\mathrm{WS}}$

$$\lambda(r, k) = \mathscr{E}_m(k) + r, \tag{5.120}$$

is given by Hamilton's equations. Remember that the phase space is $\mathrm{T}^*\mathscr{M}^*$, i.e., our configuration space is $\mathscr{M}^*$ and the momentum space is $\mathbb{R}$. Hamilton's equations become

$$\frac{\partial k}{\partial t} = \frac{\partial \lambda}{\partial r} = 1, \tag{5.121}$$

$$\frac{\partial r}{\partial t} = -\frac{\partial \lambda}{\partial k} = -\frac{\partial \mathscr{E}_m}{\partial k}. \tag{5.122}$$

This gives

$$k(t) = (t + k_0) \bmod \gamma^*, \tag{5.123}$$

$$r(t) = E - \mathscr{E}_m(t + k_0), \tag{5.124}$$

where k_0 is the initial value of $k(t)$. The period of the motion is simply $T_{\mathrm{Cl}} = \frac{2\pi}{\gamma} = \gamma^*$. The reduced action is given by

$$\mathscr{S}[E] = \int_{\Lambda(E)} \big(E - \mathscr{E}_m(k)\big)\,\mathrm{d}k = \int r \frac{\partial k}{\partial t}\,\mathrm{d}t = \int r(t)\,\mathrm{d}t, \tag{5.125}$$

which is nothing but the length of the classical trajectory (in $r-$space) or

$$\mathscr{S}[E] = E T_{\mathrm{Cl}} - \int_0^{T_{\mathrm{Cl}}} \mathscr{E}_m(t + k_0)\,\mathrm{d}t \tag{5.126}$$

$$= \gamma^* \big(E - \overline{\mathscr{E}}_m\big), \tag{5.127}$$

where $\overline{\mathscr{E}}_m$ is the mean energy over the classical path. Furthermore, we have used the definition $\gamma \cdot \gamma^* = 2\pi$. The mean energy over the classical path can also be expressed as the integral over k

$$\overline{\mathscr{E}}_m = \frac{1}{\gamma^*} \int_0^{\gamma^*} \mathscr{E}_m(k)\,\mathrm{d}k, \tag{5.128}$$

which is simply the mean energy on the band m.

The WKB ansatz in "position" coordinate (for our purposes k) corresponding to the construction of the previous sections has the form

$$\psi_{\mathrm{WKB}}(k) = \frac{\mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\mathscr{S}(k)} \psi_m^\varepsilon(k)}{\sqrt{|r(k)|}} + \mathscr{O}(\varepsilon)$$

where $\psi_m^\varepsilon(k)$ is the eigenfunction corresponding to $\lambda(r,k)=E$. We now consider the Maslov construction, i.e., we wish to determine the Maslov index μ corresponding to one revolution along the classical trajectory. If

$$E \notin \left[\min_{k\in\mathscr{M}^*} \mathscr{E}_m(k), \max_{k\in\mathscr{M}^*} \mathscr{E}_m(k)\right]$$

it is clear that $r(k)\neq 0$ (consider the solutions of Hamilton's equation of motion (5.123) and (5.124)) and hence the WKB ansatz we have written will not be singular, i.e., $\mu=0$. If

$$E \in \left[\min_{k\in\mathscr{M}^*} \mathscr{E}_m(k), \max_{k\in\mathscr{M}^*} \mathscr{E}_m(k)\right],$$

the WKB ansatz will be singular. However, the Maslov construction will give canceling contributions along the classical trajectory to the overall phase of the ansatz, i.e., $\mu=0$ (see section 4.7).

After inserting these facts into the quantization condition (5.103) we have

$$\oint \left(E-\mathscr{E}_m(k)\right) \mathrm{d}k = 2\pi\varepsilon\left(n-\frac{\gamma_\mathrm{B}}{2\pi}\right), \quad n\in\mathbb{Z}. \tag{5.129}$$

Using the above consideration on the classical dynamics, the quantization condition takes the simpler form

$$E_m^n = \overline{\mathscr{E}}_m + 2\pi\varepsilon\gamma\left(n-\frac{\gamma_\mathrm{B}\left(E_m^n\right)}{2\pi}\right), \quad n\in\mathbb{Z}. \tag{5.130}$$

We have here taken into account that the Berry term actually depends on energy, the considered band m and the index n. Note that the energies are still defined in an implicit manner.

Recall that the principal symbol $\widehat{\pi}_0$ of the almost projections $\widehat{\pi}$ are defined by the eigenfunctions of the principal symbol of $\mathscr{U}_\mathrm{BF}^{-1}\widehat{H}_\mathrm{WS}\mathscr{U}_\mathrm{BF}$, that we denoted in (5.38) as

$$\psi_m^\varepsilon(E,k,y) = \psi_m(E-r,k,y). \tag{5.131}$$

The classical evolution of r depends on the energy (see (5.124)). We can however define the variable $\rho = E-r$. We now write the Berry contribution to the integral explicitly as

$$\int_{\Lambda(E)} \left(\psi_m(E-r,k,y)\right)^* \mathrm{d}\psi_m(E-r,k,y) \tag{5.132}$$

which has to be calculated along $\Lambda(E)$. Expressed in ρ, this integral is transformed to

$$\int_{\Lambda'} \left(\psi_m(\rho, k, y)\right)^* \mathrm{d}\psi_m(\rho, k, y), \tag{5.133}$$

around Λ' described by $\big(k(t), \mathscr{E}_m(k(t))\big)$. Notice that the classical dynamics of k does not depend on the energy (and evolve over all values of $\mathscr{M}^*$, see (5.123)). We conclude that all the terms in the integral depend only on the band index m and subsequently that the Berry term is independent on the energy E. We can hence write the following quantization condition

$$E_m^n = \overline{\mathscr{E}}_m + 2\pi\varepsilon\gamma\left(n - \frac{\gamma_{\mathrm{B}}^m}{2\pi}\right), \quad n \in \mathbb{Z}, \tag{5.134}$$

where the Berry term γ_{B}^m depends only on the band index m, i.e., the energies E_m^n are up to $\mathscr{O}\big(\varepsilon^2\big)$ given explicitly. The unusual thing here is that the quantization condition (up to $\mathscr{O}\big(\varepsilon^2\big)$) describes the spectrum of a shifted energy spectrum of a harmonic oscillator! Each energy band m will result in a set of such energies. However, the shift is specific for each band and is given by the Berry phase.

5.4.2 The Wannier–Stark ladder

In the physics literature (see, e.g., the review [GKK02]), the Wannier–Stark ladder is derived by a tight–binding assumption. We describe this first in a one dimensional setting. One assumes that a specific energy band has localized states around the ℓth period of the lattice that can be build out of the eigenfunctions of the unperturbed Hamiltonian. Supposing that each lattice site has such a state and that the overlap of different states is small enough, $\widehat{H}_{\mathrm{WS}}$ can be expanded and diagonalized in this basis.

In the unperturbed case, i.e., $\varepsilon = 0$, Wannier proved the existence of exponentially localized states (Wannier states). Assuming that an energy band m to the unperturbed system has energy eigenfunctions $\psi_m(k, y)$, the Wannier state corresponding to the ℓth period of the lattice is given by

$$\psi_{m,\ell}^{\mathrm{W}} = \int_{\mathscr{M}^*} \mathrm{e}^{\mathrm{i}k\ell\gamma}\psi_m(k, y)\,\mathrm{d}k. \tag{5.135}$$

They form an orthogonal set on the subspaces spanned by the eigenstates corresponding to the energy band m. We associate here to the Wannier state ℓ of band m (which we suppress for simplicity) the ket $|\ell\rangle$ in the Dirac bra–ket notation. One important claim is that $\widehat{H}_{\mathrm{WS}}$ takes a simple form in this basis. Under

the assumption that the overlap between two Wannier states from two sites separated by at least one lattice period is small enough, the unperturbed system can be diagonalized. One finds an effective mean energy of the band $\overline{\epsilon}_m$ and an effective energy half width Δ_m such that the dispersion relation of the mth band is given by

$$\mathscr{E}_m(k) \approx \overline{\epsilon}_m + 2\Delta_m \cos\left(\frac{k}{\gamma^*}\right). \tag{5.136}$$

One can then write $\widehat{H}_{\text{WS}}$, under the tight–binding approximation, as

$$\widehat{H} = \sum_{\ell\in\mathbb{Z}} \left(\overline{\epsilon}_m + \gamma\varepsilon\ell\right) |\ell\rangle\langle\ell| + \Delta_m(|\ell+1\rangle\langle\ell| + |\ell\rangle\langle\ell+1|) \tag{5.137}$$

in the Wannier basis. This Hamiltonian can be diagonalized with eigenenergies

$$E_{(m,n)} = \overline{\epsilon}_m + 2\pi\varepsilon\gamma n,\ n\in\mathbb{Z}, \tag{5.138}$$

and eigenfunctions

$$|m,n\rangle = \sum_{j\in\mathbb{Z}} J_{j-n}\left(\frac{\Delta_m}{\varepsilon\gamma}\right)|j\rangle \tag{5.139}$$

where we have used J_l for the Bessel function (of the first kind) of order l. In this derivation, the major assumption is that the overlaps $\langle\ell\,|\ell\pm p\rangle$, $\forall\, p\geq 2$ are small enough (hence the name tight binding).

Our quantization condition renders the quasi–energies

$$E_m^n = \overline{\mathscr{E}}_m + 2\pi\varepsilon\gamma\left(n - \frac{\gamma_{\text{B}}^m}{2\pi}\right),\quad n\in\mathbb{Z}. \tag{5.140}$$

In view of (5.138), $\overline{\epsilon}_m$ is the mean energy of the energy band m so, in this respect, the two descriptions agree. The linear term in n and ε also agree. The Berry term is, however, missing in (5.138). The Wannier ladders described by (5.138) are hence only correct to $\mathscr{O}(\varepsilon)$. In theory, the fact that (5.138) is only $\mathscr{O}(\varepsilon)$ is not sufficient to state that the resonances are equidistant since the distance between the states is also $\mathscr{O}(\varepsilon)$. The fact that the Wannier–Stark resonances are equidistant to $\mathscr{O}\left(\varepsilon^2\right)$ is, however, true since the Berry term is constant for a particular band and that the quantization (5.134) delivers the energies of the resonances up to $\mathscr{O}\left(\varepsilon^2\right)$. Further note that in the case of the Wannier-Stark system all subsymbols of $\widehat{h}_{\text{BF}}^{\varepsilon}$ vanish and, hence, the corresponding term in the holonomy γ_1 also vanishes. Such terms, much like the Maslov and Berry terms, are not considered by the tight–binding approximation.

Trivially, the tight binding approximation extends to the case when the Wannier–Stark Hamiltonian is separable in d–dimensions. The WKB quantization will then reduce to solving the problem as d one dimensional systems.

The WKB quantization we rely on allows us to also include integrable motion (see 4.8). It is, however, difficult, in general, to state the exact form of the classical action involved (see (5.126)). The specific spacing of the quasi–energies is, in our description, a consequence of the fact that the action is directly proportional to the energy. It is also, in general, unclear if the Berry term will be constant for a given energy band.

Some claim in the non–separable case that one still has a certain form of Wannier–Stark ladder. For a multidimensional system with a linear perturbing potential in the direction that we denote as **u**, we find in [WKKM04], that Wannier–Stark resonance would have resonance energies

$$\mathscr{E}_{m,n}(k_{\mathrm{v}}) = \mathscr{E}_{m,0}(k_{\mathrm{v}}) + 2\pi\varepsilon n \tag{5.141}$$

where k_{v} denotes the quasi–momentum in the direction perpendicular to **u** and $\mathscr{E}_{m,0}$ a suitable dispersion relation. In the contribution of [WKKM04], the concept of separability had to be defined on the level of the operator $\widehat{H}_{\mathrm{WS}}$ on $\mathrm{L}^2(\mathbb{R}^2)$, i.e., it is equivalent to demanding the separability of the periodic potential V_Γ. The band function will then be separable as well as the corresponding classical problem with Hamiltonian $\lambda(r,k)$. We consider a non–separable but integrable Hamiltonian $\lambda(r,k)$. Formally, we do so by considering some potential $V_\Gamma(x_1,x_2)$ for which neither the potential nor the band function are integrable and a linear perturbing potential in the **1**−direction. In other words, we consider the Wannier–Stark Hamiltonian

$$\widehat{H}_{\mathrm{WS}}(\delta) = -\Delta + V_\Gamma(x_1, \delta x_2) + \varepsilon x_1. \tag{5.142}$$

In the limit $\delta \to 0$ this Hamiltonian reduces to

$$\widehat{H}_{\mathrm{WS}}(0) = \frac{\partial^2}{\partial {x_2}^2} + \left(\frac{\partial^2}{\partial {x_1}^2} + V_\Gamma(x_1, 0) + \varepsilon x_1\right), \tag{5.143}$$

which separates to a free part in the **2**−direction and a Wannier–Stark part in the **1**−direction, i.e., one would expect quasi–energies of the form

$$E_m^n = \frac{k_2^2}{2} + \overline{\mathscr{E}}_m + 2\pi\varepsilon\gamma\left(n - \frac{\gamma_{\mathrm{B}}}{2\pi}\right) + \mathscr{O}(\varepsilon^2). \tag{5.144}$$

According to (5.141) from [WKKM04], identifying the directions **1** and **2** with **u** and **v** we would have

$$\mathscr{E}_{m,n}(k_2) = \mathscr{E}_{m,0}(k_2) + 2\pi\varepsilon n \tag{5.145}$$

Obviously, the distance between the resonances does not coincide.

One could argue that to an integrable Hamiltonian $\lambda(r, k)$ we can subscribe d EBK quantization conditions

$$\mathscr{I}_i = \varepsilon\left(n_i + \frac{\mu_i}{4} - \frac{\gamma_{\mathrm{B}}}{2\pi}\right) \tag{5.146}$$

(see section 4.8) where we have included the Maslov index μ_i. This would however not imply that the resonances are discrete since we have no à priori knowledge about the resonances. For eigenvalues (see the section 4.6) we know for example that the mean spacing between eigenvalues is of order ε^{d-1}. Lacking such information for resonances, the fact that we find a discrete set of resonances does not contradict (5.141).

One should also note the contribution in [SN99] which gives a similar quantization condition for the Wannier–Stark ladder as ours. The construction is based on the effective (classical) dynamic of the center of a wave packet, i.e., it assumes that the action of the effective motion follow an EBK quantization condition where the motion is given by Peierls' substitution. The Maslov and Berry terms are included. The Berry term is incorporated by mean of a curvature term in the classical motion which yield the Berry phase.

Note that since we only consider an adiabatic transport on single energy band $\lambda(r, k)$, we cannot gain any information about the lifetimes of the so acquired resonances, i.e., we learn nothing about the imaginary part of the resonances.

5.4.3 Adiabatic propagation of localized states.

One of the aims of this thesis was the investigation of the evolution of localized states generated by $\widehat{H}_{\mathrm{WS}}$. We can do so by considering the constructed states and their quasi–energies. The WKB ansatz can be constructed at least formally to every order in ε (see section 4.7 and 5.3.1). Henceforth, we consider formally that ψ_{WKB} is an ε^∞–quasi–mode to $\widehat{H}_{\mathrm{WS}}$ for which we have calculated the quasi energies E_m^n up to order ε^2.

We denote the projection corresponding to the mth band as

$$\widehat{\Pi}_m^\varepsilon = \int_{\mathscr{M}^*}^{\oplus} \widehat{\Pi}_m^\varepsilon(k)\,\mathrm{d}k \tag{5.147}$$

where[6] $\widehat{\Pi}_m^\varepsilon = \mathrm{Op}_\varepsilon^{\mathrm{w}}[\widehat{\pi}]$ according to section 5.2.2. We can write that

$$\widehat{\Pi}_m^\varepsilon \psi_{\mathrm{WKB}} = \psi_{\mathrm{WKB}} + \mathscr{O}(\varepsilon^\infty) \tag{5.148}$$

[6] with some abuse of notation.

A result of Lemma 5.1 states that

$$\left[\mathscr{U}_{\mathrm{BF}}^{-1}\widehat{H}_{\mathrm{WS}}\mathscr{U}_{\mathrm{BF}},\widehat{\Pi}_m^{\varepsilon}\right]=\mathscr{O}(\varepsilon^{\infty}). \tag{5.149}$$

This implies that

$$\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\mathscr{U}_{\mathrm{BF}}^{-1}\widehat{H}_{\mathrm{WS}}\mathscr{U}_{\mathrm{BF}}t}\psi_{\mathrm{WKB}}\in\widehat{\Pi}_m^{\varepsilon}\mathscr{H}_{\tau},\ \forall\, t\geq 0 \tag{5.150}$$

up to errors of $\mathscr{O}(\varepsilon^{\infty})$ since ψ_{WKB} is an ε^{∞}–quasi–mode of $\widehat{H}_{\mathrm{WS}}$. We conclude that the evolution of linear combinations of such states will remain in the subspace of the mth band up to $\mathscr{O}(\varepsilon^{\infty})$.

The particular appearance of the Wannier–Stark resonances reminds us of the spectrum of the harmonic oscillator. To some extent the properties of the evolution generated by the harmonic oscillator are also valid for the Wannier–Stark system. Since the proposed WKB ansätze, this implies ψ_{WKB} are energy quasi–modes which imply in one dimension

$$\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}\mathscr{U}_{\mathrm{BF}}^{-1}\widehat{H}_{\mathrm{WS}}\mathscr{U}_{\mathrm{BF}}t}\psi_{\mathrm{WKB}}\left(E_m^n\right)=\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}E_m^n t}\psi_{\mathrm{WKB}}\left(E_m^n\right)+\mathscr{O}\left(\varepsilon^2\right), \tag{5.151}$$

where

$$E_m^n=\overline{\mathscr{E}}_m+2\pi\varepsilon\gamma\left(n-\frac{\gamma_{\mathrm{B}}^m}{2\pi}\right),\quad n\in\mathbb{Z} \tag{5.152}$$

according to (5.134). At times $T_{\mathrm{Cl}}=\gamma^*$

$$-\frac{E_m^n T_{\mathrm{Cl}}}{\varepsilon} = -2\pi\gamma\gamma^*\left(n-\frac{\gamma_{\mathrm{B}}^m}{2\pi}\right) \tag{5.153}$$

$$= -2\pi\left(n-\frac{\gamma_{\mathrm{B}}^m}{2\pi}\right), \tag{5.154}$$

since by assumption $\gamma\cdot\gamma^*=1$. Modulo 2π, this is nothing but

$$-\pi+\gamma_{\mathrm{B}}^m.$$

Any quasi–mode will under the evolution generated by $\widehat{H}_{\mathrm{WS}}$ after one classical period T_{Cl} gain a phase $-\mathrm{e}^{\mathrm{i}\gamma_{\mathrm{B}}^m}$ independently of n (modulo errors $\mathscr{O}\left(\varepsilon^2\right)$). This implies in turn that any linear combination of states ψ_{WKB} from one band m will, after T_{Cl} and to $\mathscr{O}\left(\varepsilon^2\right)$, reoccur with an additional phase $-\mathrm{e}^{\mathrm{i}\gamma_{\mathrm{B}}^m}$, i.e., the state will have a revival[7].

[7] we are careful not to use the terminology of a "classical revival" which we reserve for $\hbar$ asymptotics.

The latter is also valid for systems of higher dimension if $\lambda(k, r)$ is separable. The above argument is then simply reiterated in each direction independently. In the integrable but non–separable case, we can still associate a discrete set of quasi–energies that can be described by d relative numbers according to the EBK quantization conditions. Since the actions corresponding to these cycles on the Liouville–Arnold torus will generally not reduce to a constant times the energy (like the harmonic oscillator), the resonances will not be equidistant. It is then not possible to conclude that revivals would, in this case occur. Since the WKB ansatz relies on the integrability of the underlying classical mechanics given by the Hamiltonian $\lambda(k, r)$, we cannot make any statement in the non–integrable case.

In the case of equidistant Wannier–Stark ladders, the results of Averbukh and Perelman give us the existence of further revivals [AP89]. These authors consider equidistant eigenvalues that are slightly perturbed. This is thought to reflect quantum mechanics in the semiclassical regime. The underlying equidistant spectrum reflects classical mechanics locally whereas the perturbations reflect quantum correction. In such a case, they were able to show the existence of so–called fractional revivals. Such revivals occur at larger times scales compared to the classical period and in particular beyond the Ehrenfest time ($\hbar$ asymptotics, we refer here also to section 4.5).

5.4.4 Bloch oscillations

In view of the propagation results, we here discuss Bloch oscillations. One aim of this thesis was to shed some light on the "almost dispersionless" evolution of wave packets under the Wannier–Stark system. In particular, we made reference to the studies in [HKKM04, WKKM04] of the evolution of Gaußian wave packets.

Recent developments

We introduce the results of [HKKM04, WKKM04]. Two limiting cases were studied in these contributions. These were obtained by considering two different sets of Gaußians as initial conditions. In both cases, the Gaußians were of minimal uncertainty, i.e., the Gaußians chosen such that

$$\Delta p^2 \Delta x^2 = \frac{\hbar^2}{4} \tag{5.155}$$

(see section 4.4, (4.46)). Bloch oscillations were obtained for initial states that are sharply defined in momentum space and so–called breathing modes were obtained if the momentum distribution was broad. Breathing modes describe

wave packets whose evolved center remains at a specific point while its width oscillates in time.

In one dimension, numerical simulations were performed for initial Gaußian wave packets that were prepared such that they initially lie in the λ–eigenbundle corresponding to a single band m [HKKM04]. Up to the effects of Zener tunneling, the wave packet was reconstructed after one classical period (Bloch period). The parts of the wave packets that have tunneled to other bands evolved according to different dispersion relations. Those did however have the same period.

It was also observed that the Gaußians remained approximately of Gaußian shape up to small errors. Furthermore, for Bloch oscillations, the width of the Gaußian fluctuated relatively little when evolved which was characterized in the following manner [HKKM04]

"[...], an almost dispersionless motion of wave packets has been found."

This statement makes allusion to the fact that

- only a small part of the initial wave packet tunnels to other bands, i.e., the wave packet remains to a good approximation on the initial λ–eigenbundle,
- the wave packet remains almost dispersionless after a period of the dynamics.

The simulations were reiterated in two dimensions [WKKM04]. Many of the results of [HKKM04] found for one dimensional lattices extend to this case. The periodic potentials considered were parametrized by

$$V_\Gamma = V_0(\cos(x_1) + \cos(x_2) + \epsilon \cos(x_1)\cos(x_2)) \tag{5.156}$$

Two situations were treated. When the periodic potential was separable ($\epsilon = 0$), the oscillations in the two directions are just superimposed, i.e., they merely reflect the results found in one dimension. The wave packet reoccurs up to at most some Zener tunneling if the single Bloch oscillations in each direction reoccurs at the same time. This is the case when the classical periods of each oscillations are linearly dependent. The dispersion of the wave packet was, contrarily to one dimension, not necessarily small for Bloch oscillations. This was mostly due to Zener tunneling to higher energy bands. When comparing the projection of the evolved Gaußian, however, there was little dispersion. For a non separable potential ($\epsilon = 1$), a simulation showed the same behavior except for a larger effect of Zener tunneling which could be subscribed to smaller energy gaps between the ground band and the next energy band. The ground band of the unperturbed

Hamiltonians which were used, i.e., $\epsilon = 0, 1$, in both cases are quite close (we refer here to [WKKM04], figure 6).

In both cases, i.e., in one and two dimensions, the findings were discussed with the help of the tight binding approximation (see section 5.4.2) and formula (5.141).

Discussion

On a general footing, these numerical findings illustrate the conclusions of our findings. The two main properties we use here are the calculated Wannier–Stark resonances and the fact that we can subscribe to each energy band a set of ε^∞–quasi–modes which is invariant under the evolution generated by $\widehat{H}_{\mathrm{WS}}$. Any linear combinations of these ε^∞–quasi–modes given by the quantization procedure, will remain in the subspace of the mth energy band to $\mathcal{O}(\varepsilon^\infty)$ when evolved under $\widehat{H}_{\mathrm{WS}}$. Hence, the projection of an initial state onto the subspace spanned by the ε^∞–quasi modes of a band m will remain in that band to $\mathcal{O}(\varepsilon^\infty)$. For these states, the evolution is given by the Wannier–Stark resonances to $\mathcal{O}\left(\varepsilon^2\right)$.

In one dimension, the resonances are equidistant to $\mathcal{O}\left(\varepsilon^2\right)$, revivals will hence occur for linear combinations of the ε^∞–quasi–modes. This is the case numerically whether the initial Gaußian on one band describes a breathing mode or a Bloch oscillation. In fact, our considerations show that this is the case for any linear combination of the constructed states. This also applies to higher dimensional systems.

In $d > 1$, our construction produces (for a given band) one Wannier–Stark ladder per lattice dimension if the system is integrable. If the system is separable, we find that d quantization conditions that each produce resonances that are arranged equidistantly. If the periods of each separated Bloch oscillation are linearly dependent, again, revivals will occur to $\mathcal{O}\left(\varepsilon^2\right)$. In this respect, our findings agree with those of [WKKM04].

For the integrable but not separable case, the resonances will not, in general, be equidistant to $\mathcal{O}\left(\varepsilon^2\right)$, i.e., one would expect that an initial state on that band would disperse under the evolution generated by $\widehat{H}_{\mathrm{WS}}$. We would be tempted to state that the simulated similarity between the separable and non-separable cases (i.e., $\epsilon = 0$ and $\epsilon = 1$) are not typical. This is further sustained by the fact that the unperturbed dispersion relation for the energy band are very similar (again see [WKKM04], figure 6). If the band functions are close, it is likely that the quantization of the corresponding classical motion render similar quasi–energies. This could explain the similarity. In other words, the $\epsilon = 1$ case can be considered as a small perturbation of the $\epsilon = 0$ case, when considering the classical motion generated by the ground energy band of the principal symbol

of $\widehat{H}_{\mathrm{WS}}$.

Appendix A

The symplectic group $\mathrm{Sp}(2d)$

We consider here some properties of the (real) symplectic group $\mathrm{Sp}(2d, \mathbb{R})$, i.e., the group represented by the real $2d \times 2d$ matrices (with matrix multiplication) of the general linear group $\mathrm{GL}(2d, \mathbb{R})$. The results are taken from [Fol89].

Definition A.1. The symplectic group is the group of matrices in $\mathrm{GL}(2d, \mathbb{R})$ that satisfy

$$\mathscr{J} = S^T \mathscr{J} S \tag{A.1}$$

where

$$\mathscr{J} = \begin{pmatrix} 0 & -\mathbb{1}_{d\times d} \\ \mathbb{1}_{d\times d} & 0 \end{pmatrix} \tag{A.2}$$

is the symplectic unity.

One can characterize the symplectic group in the following manner.

Corollary A.1. *Let* $S = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \in \mathrm{GL}(2d, \mathbb{R})$. *The following statements are equivalent:*

- $S \in \mathrm{Sp}(d, \mathbb{R})$,
- $S^T \in \mathrm{Sp}(d, \mathbb{R})$,
- $S^{-1} = \mathscr{J} S^T \mathscr{J}^{-1} = \begin{pmatrix} \delta^T & -\beta^T \\ -\gamma^T & \alpha^T \end{pmatrix}$.

Lemma A.1. *The symplectic group is generated by the matrices*

$$\begin{pmatrix} \alpha & 0 \\ 0 & (\alpha^{-1})^T \end{pmatrix}, \quad \begin{pmatrix} \mathbb{1}_{d\times d} & \beta \\ 0 & \mathbb{1}_{d\times d} \end{pmatrix}, \quad \mathscr{J}, \tag{A.3}$$

where $\alpha \in \mathrm{GL}(d, \mathbb{R})$ *and* β *is symmetric.*

The corollary implies that $\det(S) \neq 0$. In particular, this leads to the following property for the singular values.

Lemma A.2. *If* λ *is a singular value of* $S \in \mathrm{Sp}(d, \mathbb{R})$*, then* $\frac{1}{\lambda}$ *will also be a singular value.*

Appendix B

The metaplectic representation

The aim here is to give a short introduction and some results to the metaplectic representation. For proofs, again see [Fol89].

A natural object to consider in this context is the Heisenberg Lie algebra $\mathfrak{h}_d$ here represented by the matrices

$$m(p;q;t)=\begin{pmatrix} 0 & p & t \\ 0 & 0_{d\times d} & q \\ 0 & 0 & 0 \end{pmatrix}\in\mathfrak{h}_d,\quad p\in\mathbb{R}^d, q\in\mathbb{R}^d. \tag{B.1}$$

The corresponding Lie group, the Heisenberg group $\mathbb{H}_d$ is represented by the matrices

$$M(p;q;t)=\mathbb{1}_{(d+2)\times(d+2)}+m(p;q;t) \tag{B.2}$$

We name the following elements of $\mathfrak{h}_d$

$$P_j=m\big(0,...,p_j,...,0;0;0\big),\ Q_j=m\big(0;0,...,q_j,...,0;0;0\big),\ T=m(0;0;t),$$

which are nothing but a basis of $\mathbb{R}^{2d+1}$. The Lie algebra $\mathfrak{h}_d$ is given by

$$\big[m(p;q;t),m(p';q';t)\big]=m\big(0;0;\big[(p,q),(p',q')\big]\big) \tag{B.3}$$

where $[(p,q),(p',q')]$ is the commutator $pq'-p'q$. Insertion gives

$$\big[P_j,P_k\big]=\big[Q_j,Q_k\big]=\big[P_j,T\big]=\big[Q_j,T\big]=0,\quad \big[P_j,Q_k\big]=\delta_{jk}T \tag{B.4}$$

which are isomorphic to the commutation relations for momentum and position observables of classical (Poisson bracket) and quantum mechanics.

We need a unitary representation of the Heisenberg group on $\mathrm{L}^2\big(\mathbb{R}^d\big)$. The map

$$m(p;q;t)\mapsto\frac{\mathrm{i}}{\hbar}\big(q\widehat{p}-p\widehat{x}+t\mathbb{1}\big) \tag{B.5}$$

is a homomorphism from $\mathfrak{h}_d$ to skew Hermitian operators on $\mathcal{S}\left(\mathbb{R}^d\right)$. The exponential map

$$\widehat{\mathscr{T}}(p,q)=\exp\left(\frac{\mathrm{i}}{\hbar}(q\widehat{p}-p\widehat{x})\right). \tag{B.6}$$

gives a unitary projective representation of the Heisenberg group (none other than the translation operator given in section 4.3.2). We disregard the phase terms $\mathrm{e}^{\frac{\mathrm{i}}{\hbar}t}$ which do not play a role in practice.

Theorem B.1 (Stone–von Neuman)**.** *Let $\hbar\neq 0$. Then every unitary irreducible representation of $\mathbb{H}_d$ is equivalent to either $\widehat{\mathscr{T}}$ acting on $\mathrm{L}^2\left(\mathbb{R}^d\right)$ or $\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(ap+bq)}$, $(a,b)\in\mathbb{R}^d$ acting on $\mathbb{C}$.*

Now, let S be a linear symplectomorphism on $\mathrm{T}^*\mathbb{R}^d$. It is easily seen that a map $\mathbb{R}^{2d+1}\to\mathbb{R}^{2d+1}$, $(p;q;t)\mapsto(S(p,q),t)$ is an automorphism. $\widehat{\mathscr{T}}\left(S^{-1}X\right)$ will also be a unitary representation of the Heisenberg group if $\widehat{\mathscr{T}}(X)$ is one. Hence, these two representations are unitarily equivalent. Hence, there exists a unitary operator $\widehat{\mathscr{M}}[S]$ such that

$$\widehat{\mathscr{T}}\left(S^{-1}X\right)=\widehat{\mathscr{M}}[S]^{-1}\,\widehat{\mathscr{T}}(X)\widehat{\mathscr{M}}[S]. \tag{B.7}$$

Moreover, by Schur's Lemma (see [Fol89]) we may write

$$\widehat{\mathscr{M}}[S_1S_2]=\mathrm{e}^{\mathrm{i}u(S_1,S_2)}\widehat{\mathscr{M}}[S_1]\,\widehat{\mathscr{M}}[S_2]. \tag{B.8}$$

Actually, it is possible to show that the phase $\mathrm{e}^{\mathrm{i}u(S_1,S_2)}$ can be chosen as ±1. So, the metaplectic representation forms a double valued unitary representation of the linear symplectomorphisms of $\mathrm{T}^*\mathbb{R}^d$.

Proposition B.1. *If $S\in\mathrm{Sp}(d,\mathbb{R})$, the operator $\widehat{\mathscr{M}}[S]$ maps $\mathcal{S}\left(\mathbb{R}^d\right)$ isomorphically onto itself and extends by continuity to an isomorphism of $\mathcal{S}'\left(\mathbb{R}^d\right)$.*

In particular if $\psi\in\mathcal{S}\left(\mathbb{R}^d\right)$, the following can be verified

$$\widehat{\mathscr{M}}\left[\begin{pmatrix}\alpha & 0\\ 0 & (\alpha^{-1})^T\end{pmatrix}\right]\psi(x) = \sqrt{\det(\alpha)}\psi\left(\alpha^T x\right), \tag{B.9}$$

$$\widehat{\mathscr{M}}\left[\begin{pmatrix}\mathbb{1}_{d\times d} & \beta\\ 0 & \mathbb{1}_{d\times d}\end{pmatrix}\right]\psi(x) = \pm\exp\left(\frac{\mathrm{i}}{2\hbar}x\beta x\right)\psi(x), \tag{B.10}$$

$$\widehat{\mathscr{M}}[\mathscr{J}]\left(\mathscr{F}_\hbar\psi\right)(\xi) = \mathrm{i}^{\frac{d}{2}}\left(\mathscr{F}_\hbar\psi\right)(\xi), \tag{B.11}$$

where $\mathscr{F}_\hbar$ is the usual $\hbar-$Fourier transform of quantum mechanics.

A special case of the above equalities gives the evolution of a (squeezed) Gaußian state under the action of the quantization of a linear (possibly time dependent) symplectomorphism. i.e., the evolution generated by a quadratic Hamiltonian. These properties are used to calculate the evolution of the squeezed states of section 4.3.2. Note that a Gaußian shape remains a Gaußian shape under the action of the quantization of all linear symplectomorphisms. We remind that the group of linear symplectic matrices is generated by the matrices in (B.9), (B.10) and (B.11) (see appendix A, Lemma A.1).

Zusammenfassung

Der Gegenstand dieser Arbeit ist die Untersuchung der Eigenschaften von gestörten periodischen Quantensystemen. Dies wird mit Hilfe von Methoden der Semiklassik durchgeführt, d.h. durch asymptotische Betrachtungen, die einen Zusammenhang zwischen Quantenmechanik und klassischer Mechanik herstellen. Ferner werden gestörte periodische Schrödingeroperatoren studiert.

Der erste Teil dieses Arbeit führt die nötigen Werkzeuge ein. Insbesondere wird die Floquet Theorie behandelt anhand des Beispiels einer linearen Differentialgleichung zweiter Ordnung. Solche Differentialgleichungen treten beispielsweise in der Spektraltheorie von periodischen Schrödingeroperatoren auf. Hier wird die Mathieu'sche Differentialgleichung betrachtet und insbesondere die Eigenschaften ihrer Eigenwerte. Jede Floquet Lösung der Differentialgleichung besitzt eine charakteristische Zahl: den Floquet–Exponenten. Von allgemeinenem Interesse ist die Beziehung zwischen den Eigenwerten und den Floquet–Exponenten. Diese Beziehung wird durch die Whittaker–Hill–Gleichung beschrieben. Diese Gleichung ist bekannt bis auf die Determinante einer unendlich dimensionalen Matrix. Unsere Resultate geben eine explizite Darstellung für diese Determinante und zwar als den Limes einer Rekursion dritter Ordnung. Wir geben ein Verfahren an, um jede lineare Rekursion ohne konstante Terme aufzusummieren. Damit ist jeder Term in der Whittaker–Hill–Gleichung explizit angegeben.

Da wir uns mit semiklassischen Methoden beschäftigen, führen wir die klassische Mechanik ein. Danach führen wir die Weyl–Quantisierung ein. Diese Theorie stellt einen klaren Zusammenhang zwischen der klassischen und der Quantenmechanik her. Unter anderem ermöglicht sie, approximative Lösungen zur quantenmechanischen Zeitentwicklung anzugeben [CR97]. Diese approximativen Lösungen verwenden klassische Größen und geben die Zeitentwicklung von Wellenpaketen mit Gaußschen Profilen als Anfangswert an. Wir benutzen diese Resultate, um weitere Eigenschaften von zeitentwickelten Wellenpaketen zu untersuchen. Wir können zeigen, daß ein Wellenpaket lokalisiert bleibt, wenn die Hesse–Matrix der zugehörigen klassischen Hamilton–Funktion eine Floquet Lösung annimmt. Weiter kann in diesem Fall das so genannte klas-

sische Wiederkehrphänomen vorkommen.

Der letzte Teil ist dem Studium der Spektren von periodischen Schrödingeroperatoren gewidmet. Auch hier benützen wir semiklassische Methoden. Diese werden jedoch im Störungsparameter durchgeführt und nicht wie üblich in $\hbar$. Um die Semiklassik zu benutzen, müssen wir eine operatorwertige klassische Mechanik betreiben. Dies wird im Kontext von τ–equivarianten Symbolen realisiert [PST03]. Hierfür benutzen wir frühere Resultate über die Spektren von gestörten periodischen Schrödingeroperatoren. Insbesondere ist bekannt, daß das Spektrum solcher Operatoren absolut stetig bleibt und in Bändern auftritt [CH91]. Dies erlaubt eine adiabatische Behandlung des Problems und insbesondere eine effektive Beschreibung der Zeitentwicklung auf dem Unterraum eines Energiebandes. Durch einen WKB–Ansatz finden wir eine Einstein–Brillouin–Keller–Quantisierungsbedingung, die die Energie von Resonanzen bis auf Fehler von $\mathcal{O}(\varepsilon^2)$ beschreibt, die im absolut stetigen Spektrum eingebettet sind. Zunächst werden periodische Schrödingeroperatoren studiert, die nur mit linearen Termen gestört werden, so genannten Wannier–Stark–Resonanzen. Wir benutzen die beschriebenen Resonanzen, um die Zeitentwicklung von Wellenpaketen zu charakterisieren. Wenn das System separabel ist, folgt, daß es für jede Dimension und jedes Energieband eine Folge von equidistanten Resonanzen gibt. Dies ist möglich, da geometrische Terme, wie der Berry–Term in der Einstein–Brillouin–Keller–Quantisierungsbedingung, konstant für ein gewisses Energieband ist. In Analogie zum harmonischen Oszillator folgt dann, daß Wiederkehrphänomene auftreten und daß die Effekte des Tunnelns klein sind. Auch die Ergebnisse von früheren numerischen Untersuchungen werden diskutiert [HKKM04, WKKM04].

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Erklärung

Hiermit versichere ich, daß ich die vorliegende Arbeit selbständig angefertigt und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt habe, sowie die Wörtlich oder inhaltlich übernommenen Stellen als solche kenntlich gemacht habe.

Ulm, den 23 October, 2008

Jan Eric Sträng

Appendix C

Notation

$\mathbb{N}$	natural numbers	
$\mathbb{N}_0$	$\mathbb{N} \cup \{0\}$	
$\mathbb{Z}$	relative numbers	
$\mathbb{Q}$	rational numbers	
$\mathbb{R}$	real numbers	
$\mathbb{C}$	complex numbers	
$\mathbb{T}^N$	$N-$torus	
i	complex unity	
$\mathscr{J}$	symplectic unity	Def. A.1
$\mathrm{Mn}(N, \mathbb{X})$	group of $N \times N$ matrices with entries in $\mathbb{X} = \mathbb{R}$ or $\mathbb{X} = \mathbb{C}$	
$\mathrm{GL}(N, \mathbb{X})$	set of invertible matrices in $\mathrm{Mn}(N, \mathbb{X})$	
$\mathrm{SL}(N, \mathbb{X})$	set of matrices in $\mathrm{GL}(N, \mathbb{X})$ with determinant 1	
$\mathrm{Sp}(N)$	set of symplectic $N \times N$ matrices	Def. A.1
$\mathrm{O}(N)$	set of orthogonal $N \times N$ matrices	
$\mathrm{U}(N)$	set of unitary $N \times N$ matrices	
$\mathrm{SU}(N)$	set of unitary matrices with determinant 1	
Σ_N	Siegel upper half space of matrices in $\mathrm{Mn}(N, \mathbb{C})$	4.3.1
$\mathbb{H}_N$	the Heisenberg group of dimension N	App. B
$\mathfrak{h}_N$	the Heisenberg Lie algebra of dimension N	App. B
$\mathrm{L}^2(\mathbb{X})$	space of square integrable functions on $\mathbb{X}$	
$\mathrm{L}^k(\mathbb{X})$	space of functions whose k^{th} power is integrable on $\mathbb{X}$	

$\mathrm{L}^2_{\mathrm{loc}}(\mathbb{X})$	space of locally square integrable functions on $\mathbb{X}$	
$\mathrm{C}^k(\mathbb{X})$	the space of k–times differentiable functions whose k derivatives are continuous	2.1
$\mathrm{C}^\infty(\mathbb{X})$	the space of smooth functions over $\mathbb{X}$	
$\mathcal{S}(\mathbb{X})$	space of Schwartz test functions on $\mathbb{X}$	4.1
$\mathcal{S}'(\mathbb{X})$	space of linear forms on $\mathcal{S}(\mathbb{X})$	
$\{f, g\}$	Poisson bracket	3.1
$\mathscr{J}$	symplectic identity	3.1
$\mathrm{sgn}(X)$	number of negative eigenvalues of the matrix X	4.7
$\mathrm{T}^*\mathbb{X}$	cotangent bundle of manifold $\mathbb{X}$	
$\mathrm{T}_x\mathbb{X}$	tangent space of a manifold $\mathbb{X}$ at a point x	
$\mathrm{T}\mathbb{X}$	tangent bundle of a manifold $\mathbb{X}$	
$\mathscr{L}_X$	Lie derivative along a flow generated by the vector field X	
S_m	symbol class of order m	4.1
$\mathrm{S}^{\mathrm{Cl}}_m$	symbol class of classical symbols of order m	4.1
f_ϵ	function with asymptotic expansion in ϵ	4.1
$\mathrm{symb}^{\mathrm{w}}_{\epsilon,n}\left[\widehat{X}\right]$	ϵ–Weyl subsymbol of order n of the operator $\widehat{X}$	4.2
$f_\epsilon \sharp\!\!\sharp_\epsilon g_\epsilon$	ϵ–Moyal product of the functions f_ϵ and g_ϵ	4.3
$[h_\epsilon, f_\epsilon]_{\sharp\!\!\sharp,\epsilon}$	ϵ–Moyal commutator of the functions f_ϵ and g_ϵ	4.3
$\mathrm{Op}^{\mathrm{w}}_\epsilon[f_\epsilon]$	ϵ–Weyl quantization of the function f_ϵ	4.1
$\mathscr{F}$	Fourier transform	
$\mathscr{U}_{\mathrm{BF}}$	Bloch-Floquet transform	5.1.1
$\mathscr{B}(\mathscr{H}_0, \mathscr{H}_1)$	space of bounded operators from $\mathscr{H}_0$ to $\mathscr{H}_1$	

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