ULM-TP/00-1
April 2000

Quantum ergodicity for Pauli Hamiltonians with spin 1/2

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Abstract

Quantum ergodicity, which expresses the semiclassical convergence of almost all expectation values of observables in eigenstates of the quantum Hamiltonian to the corresponding classical microcanonical average, is proven for non-relativistic quantum particles with spin 1/2. It is shown that quantum ergodicity holds, if a suitable combination of the classical translational dynamics and the spin dynamics along the trajectories of the translational motion is ergodic.

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1 Introduction

In quantum chaos one is primarily interested in statistical properties of eigenvalues and eigenvectors of quantum Hamiltonians whose classical limits generate chaotic dynamics. In this context the eigenvalue statistics on the scale of the mean level spacing are expected to be described by random matrix theory (see, e.g., [BGS84, Meh91]). This conjecture has since found overwhelming confirmation, mostly based on numerical calculations of eigenvalues in many systems. For the corresponding eigenvectors one also expects a random behaviour, and various tools to measure this have been invented. Among them one finds one of the few results in quantum chaos for which a mathematical proof is available: if a classical system is ergodic, its quantum mechanical counterpart is quantum ergodic. By this one understands a semiclassical convergence of almost all phase-space lifts of eigenfunctions of the Hamiltonian (e.g., their Wigner- and Husimitransforms) towards equidistribution with respect to microcanonical (i.e. Liouville) measure. One thus has obtained a realisation of the semiclassical eigenfunction hypothesis (see, e.g., [Ber83]) for classically ergodic systems.

Quantum ergodicity was first established for the free motion of a particle on a compact Riemannian manifold, where the quantum dynamics is generated by minus the Laplace-Beltrami operator on that manifold. This goes back to Shnirelman [Shn74], and the first complete proofs are due to Zelditch [Zel87] and Colin de Verdière [CdV85]. In the systems considered by these authors the semiclassical limit is actually realised as a high-energy limit. However, for Schrödinger operators involving a potential and possibly also a magnetic field the semiclassical limit can in general only be performed in terms of $\hbar \to 0$. In this setting quantum ergodicity was first proven by Helffer, Martinez, and Robert [HMR87]. All of the work mentioned so far exclusively dealt with the dynamics of point particles without internal degrees of freedom; in particular no spin was involved. On the level of the quantum Hamiltonians $\hat{H}$ that were taken into account, this is reflected in the fact that $\hat{H}$ appears as a (Weyl-) quantisation of a scalar symbol. The only degrees of freedom appearing are therefore those that possess a direct classical analogue. These are in fact the translational degrees of freedom, which on the classical side yield as a phase space a smooth symplectic manifold that in typical cases is the cotangent bundle over the configuration manifold. In this setting internal degrees of freedom would appear through the fact that the quantum mechanical observables are quantisations of matrix valued symbols, such that the vector spaces these matrices operate on represent the internal degrees of freedom.

In quantum mechanics internal degrees of freedom often arise due to the presence of symmetries. Since in general symmetries have to be implemented through (anti-) unitary representations of the respective symmetry groups on the Hilbert space of state vectors, representations of dimensions exceeding one introduce discrete degrees of freedom. It then can happen that these additional degrees of freedom do not possess classical analogues. A prominent example of this phenomenon is provided by the spin of a particle, which arises through the space-time symmetries that either form the Lorentz group (in a relativistic theory), or the Galilei group (in a non-relativistic theory). Both these symmetry groups contain the proper rotations, i.e. SO(3), as a subgroup. Through the unitary projective representations of the Lorentz or Galilei group, respectively, which implement the space-time symmetries in the quantum theory, one therefore introduces the unitary irreducible representations of $\mathrm{Spin}\,(3) = \mathrm{SU}(2)$, i.e. spin. On the classical side the rotation group, however, remains to be $\mathrm{SO}(3)$, which then enters in terms of spatial angular momentum. There exists, however, no direct classical analogue of spin. Coming back now to the problem of quantum ergodicity for particles with spin, there immediately arises the question for a criterion to be imposed on the classical system in order to ensure that the eigenfunctions of the quantum Hamiltonian behave quantum ergodically in the semiclassical limit. We recall that in the case without spin such a criterion was given by the ergodicity of the dynamics on the classical phase space with respect to Liouville measure. One would now expect that the presence of additional, internal degrees of freedom requires an extended criterion in order that quantum ergodicity holds.

It is the primary goal of the present work to elaborate on this question in some detail for the case of a non-relativistic quantum particle with spin 1/2. Our proof of quantum ergodicity in this context generalises the methods of [Shn74, Zel87, CdV85, HMR87] to the situation of Weyl operators with 2×2-matrix valued symbols. This requires two essential ingredients. The first one is an Egorov Theorem, which relates the semiclassical limit of the quantum mechanical time evolution of an observable to the classical time evolution of the corresponding classical observable. The second input required is a Szegö limit formula, which expresses the semiclassical limit of averaged expectation values of observables in eigenstates of the Hamiltonian in terms of a classical microcanonical average. In the course of the subsequent proof of quantum ergodicity we primarily rely on the method developed in [Zel96, ZZ96], which provides a considerable simplification over the original proofs given in [Zel87, CdV85, HMR87]. Already the Egorov property that one encounters for systems with spin hints at the construction that yields the 'classical' criterion for quantum ergodicity that we seek for. It leads us to consider an $\mathrm{SU}(2)$-extension of the Hamiltonian flow that arises from the classical limit of the translational degrees of freedom. The thus extended flow is defined on a product phase space that consists of two parts: the translational part is the hypersurface of fixed energy in the classical phase space, whereas the spin part is given by the group manifold of $\mathrm{SU}(2)$. The translational part of the combined dynamics is then provided by the Hamiltonian flow. The latter also drives the spin dynamics that takes place on $\mathrm{SU}(2)$ and consists of a left multiplication by a spin transport matrix, which propagates the spin degrees of freedom along the trajectories of the Hamiltonian flow. Our main result, stated in Theorem 4.1, then is that ergodicity of the combined flow is a sufficient criterion for quantum ergodicity. At this point we remark that the problem of quantum ergodicity for quantisations of matrix valued symbols was already considered in [Zel96] as an example for the general theory of quantum ergodicity of C^* dynamical systems. There it was, however, overlooked that in the relevant Egorov Theorem, apart from a transport by the Hamiltonian flow, the principal symbol of an observable is also conjugated with the spin transport matrices. As a consequence, the result stated in [Zel96] is hence incorrect, to the extent that ergodicity of the Hamiltonian flow alone is insufficient to guarantee quantum ergodicity. In section 5 we give an example that illustrates this fact.

This paper is organised as follows. In section 2 we review some background on $\hbar$-pseudodifferential calculus and define the type of Hamiltonians and observables that will be considered in the sequel. The two major ingredients required for quantum ergodicity, namely the Egorov property and the Szegö limit formula, are developed in section 3. Our main result, quantum ergodicity for Pauli Hamiltonians with spin 1/2, is then proven in section 4. Finally, in section 5 we discuss the consequences of quantum ergodicity for Wigner- and Husimitransforms of eigenfunctions and, furthermore, give an example that illustrates why ergodicity of the Hamiltonian flow alone is not a sufficient criterion for quantum ergodicity.

2 Semiclassical background

In non-relativistic quantum mechanics the dynamics of a particle with spin $s \in \frac{1}{2}\mathbb{N}$ is governed by the Pauli equation

$$\mathrm{i}\hbar \frac{\partial \psi}{\partial t}(\boldsymbol{x}, t) = \hat{H}_P \psi(\boldsymbol{x}, t) \tag{2.1}$$

with the quantum Hamiltonian

$$\hat{H}_P = \hat{H}_{trans.} \mathbb{1}_{2s+1} + \hbar\, \boldsymbol{\Sigma} \cdot \hat{\boldsymbol{C}} \tag{2.2}$$

acting as a self-adjoint operator on a suitable domain in the Hilbert space $L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2s+1}$. Here

$$\hat{H}_{trans.} = \frac{1}{2m} \left(\frac{\hbar}{\mathrm{i}} \boldsymbol{\nabla}_x - \frac{e}{c} \boldsymbol{A}(\boldsymbol{x}) \right)^2 + e\varphi(\boldsymbol{x}) \tag{2.3}$$

describes the dynamics of the translational degrees of freedom of a spinning particle with mass m and charge e which is subject to external electromagnetic forces generated by the (static) potentials $\boldsymbol{A}$ and φ. Furthermore, the components Σ_k, $k = 1, 2, 3$, of $\boldsymbol{\Sigma}$ denote the hermitian generators of the Lie algebra su(2) in the (irreducible) spin-s representation, which is of dimension $2s+1$. The coupling of the spin degrees of freedom to the translational ones is provided by the operators $\hat{C}_k$, which are suitable quantisations of functions $C_k(\boldsymbol{p}, \boldsymbol{x})$ on phase space. The latter can, e.g., describe a coupling to an external magnetic field, $\boldsymbol{C}_B(\boldsymbol{p}, \boldsymbol{x}) = -\frac{e}{2mc} \boldsymbol{B}(\boldsymbol{x})$, or a spin-orbit coupling $\boldsymbol{C}_{\mathrm{so}}(\boldsymbol{p}, \boldsymbol{x}) = \frac{1}{4m^2c^2|\boldsymbol{x}|} \frac{\mathrm{d}\varphi(|\boldsymbol{x}|)}{\mathrm{d}|\boldsymbol{x}|} (\boldsymbol{x} \times \boldsymbol{p})$.

Here, and in the following, we choose all quantum mechanical observables to be Weyl quantisations of matrix valued symbols. In general this is defined for $B \in \mathcal{S}'(\mathbb{R}^d \times \mathbb{R}^d) \otimes \mathbb{C}^{n\times n}$ and $\psi \in \mathcal{S}(\mathbb{R}^d) \otimes \mathbb{C}^n$ as

$$(\hat{B}\psi)(x) := \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathrm{e}^{\frac{\mathrm{i}}{\hbar} \boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})}\, B\Big(\boldsymbol{p}, \frac{1}{2}(\boldsymbol{x}+\boldsymbol{y})\Big)\, \psi(\boldsymbol{y})\, \mathrm{d}y\, \mathrm{d}p\ , \tag{2.4}$$

where $\hbar \in (0, \hbar_0]$ serves as a parameter. The quantisation (2.4) yields a continuous map from $\mathcal{S}(\mathbb{R}^d) \otimes \mathbb{C}^n$ to $\mathcal{S}'(\mathbb{R}^d) \otimes \mathbb{C}^n$. However, in order to obtain a semiclassical calculus one has to restrict attention to smaller classes of symbols and operators. In particular, one wishes to consider operators that can be composed with one another, e.g., operators which map $\mathcal{S}(\mathbb{R}^d)\otimes\mathbb{C}^n$ into itself. In defining suitable symbol classes we use the following notion, which is in accordance with [DS99]:

A function $m : \mathbb{R}^d \times \mathbb{R}^d \to (0,\infty)$ is called an *order function*, if there are constants $C_0 > 0,\ N_0 > 0$ such that

$$m(\boldsymbol{p},\boldsymbol{x}) \leq C_0 \sqrt{1+(\boldsymbol{p}-\boldsymbol{q})^2+(\boldsymbol{x}-\boldsymbol{y})^2}^{N_0}\ m(\boldsymbol{q},\boldsymbol{y}) \ . \tag{2.5}$$

An example for such an order function is

$$m(\boldsymbol{p},\boldsymbol{x}) = 1+\boldsymbol{p}^2+\boldsymbol{x}^2 \ . \tag{2.6}$$

Definition 2.1. Let m be an order function on $\mathbb{R}^d\times\mathbb{R}^d$. We define the symbol class $\mathrm{S}(m)$ to be the set of $B \in C^\infty(\mathbb{R}^d\times\mathbb{R}^d)\otimes\mathbb{C}^{n\times n}$ such that for every $\alpha,\beta\in\mathbb{N}_0^d$ there exists $C_{\alpha,\beta}>0$ with

$$\|\partial_p^\alpha\partial_x^\beta B(\boldsymbol{p},\boldsymbol{x})\| \leq C_{\alpha,\beta}\, m(\boldsymbol{p},\boldsymbol{x}) \ , \tag{2.7}$$

where $\|\cdot\|$ is some (arbitrary) matrix norm on $\mathbb{C}^{n\times n}$.

If $B = B(\boldsymbol{p},\boldsymbol{x};\hbar)$ depends on $\hbar\in(0,1]$, we say that $B\in\mathrm{S}(m)$, if $B(\cdot,\cdot;\hbar)$ is uniformly bounded in $\mathrm{S}(m)$ when $\hbar$ varies in $(0,1]$. For $k\in\mathbb{R}$ we let $\mathrm{S}^k(m)$ be the set of functions $B(\boldsymbol{p},\boldsymbol{x};\hbar)$ on $\mathbb{R}^d\times\mathbb{R}^d\times(0,1]$ that belong to $\hbar^{-k}\mathrm{S}(m)$ and satisfy

$$\|\partial_p^\alpha\partial_x^\beta B(\boldsymbol{p},\boldsymbol{x};\hbar)\| \leq C_{\alpha,\beta}\, m(\boldsymbol{p},\boldsymbol{x})\,\hbar^{-k} \ . \tag{2.8}$$

A sequence of symbols $B_j\in\mathrm{S}^{k_j}(m)$, with $k_j\to-\infty$ monotonically, defines an asymptotic expansion of $B\in\mathrm{S}^{k_0}(m)$, denoted by

$$B \sim \sum_{j=0}^{\infty} B_j \ , \tag{2.9}$$

if

$$B - \sum_{j=0}^{N} B_j \in \mathrm{S}^{k_{N+1}}(m) \tag{2.10}$$

for every $N\in\mathbb{N}_0$. We will often use the smaller class of *classical symbols* $\mathrm{S}^k_{\mathrm{cl}}(m)$, whose elements $B\in\mathrm{S}^k_{\mathrm{cl}}(m)$ possess asymptotic expansions in integer powers of $\hbar$, i.e.

$$B \sim \sum_{j=0}^{\infty}\hbar^{-k+j}B_j \ , \qquad B_j\in\mathrm{S}(m) \ . \tag{2.11}$$

In all of the above symbol classes the composition of the corresponding Weyl operators is well defined in the following sense (see, e.g., [DS99]):

Lemma 2.2. *Let m_1, m_2 be order functions. For $B_j \in \mathrm{S}(m_j)$ the product of the associated Weyl operators reads in terms of their symbols*

$$\hat{B}_1 \hat{B}_2 = \widehat{B_1 \# B_2} \ , \tag{2.12}$$

where $(B_1, B_2) \mapsto B_1 \# B_2$ is a bilinear continuous map from $\mathrm{S}(m_1) \times \mathrm{S}(m_2)$ to $\mathrm{S}(m_1 m_2)$. It is explicitly given by

$$(B_1 \# B_2)(\boldsymbol{p}, \boldsymbol{x}) = e^{\frac{i\hbar}{2}\sigma(\partial_p, \partial_x; \partial_q, \partial_y)} B_1(\boldsymbol{p}, \boldsymbol{x}) \, B_2(\boldsymbol{q}, \boldsymbol{y})\Big|_{\substack{\boldsymbol{q}=\boldsymbol{p} \\ \boldsymbol{y}=\boldsymbol{x}}} \ , \tag{2.13}$$

where $\sigma(\boldsymbol{v}_p, \boldsymbol{v}_x; \boldsymbol{w}_p, \boldsymbol{w}_x) := \boldsymbol{v}_x \cdot \boldsymbol{w}_p - \boldsymbol{v}_p \cdot \boldsymbol{w}_x$ denotes the symplectic two-form on $\mathbb{R}^d \times \mathbb{R}^d$. Furthermore, the asymptotic expansion of (2.13) in $\mathrm{S}(m_1 m_2)$ reads

$$(B_1 \# B_2)(\boldsymbol{p}, \boldsymbol{x}) \sim \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{i\hbar}{2} \sigma(\partial_p, \partial_x; \partial_q, \partial_y) \right)^k B_1(\boldsymbol{p}, \boldsymbol{x}) \, B_2(\boldsymbol{q}, \boldsymbol{y}) \Bigg|_{\substack{\boldsymbol{q}=\boldsymbol{p} \\ \boldsymbol{y}=\boldsymbol{x}}} \ . \tag{2.14}$$

The Pauli Hamiltonians (2.2) that we are going to study below can be viewed as Weyl quantisations of hermitian symbols $H \in \mathrm{S}^0_{\mathrm{cl}}(m)$, where m is an order function with $m \geq 1$. The symbol H then has an asymptotic expansion of the type (2.11),

$$H \sim \sum_{j=0}^{\infty} \hbar^j H_j \ , \qquad H_j \in \mathrm{S}(m) \ , \tag{2.15}$$

and the principal symbol H_0 is supposed to be a scalar multiple of $\mathbb{1}_n$, i.e. $H_0 = H_{0,s} \mathbb{1}_n$. Since in quantum mechanics Hamilton operators must be self-adjoint and bounded from below, we require the real valued function $H_{0,s}$ to fulfill the following properties:

1. $H_{0,s}$ is bounded from below.
2. There exists an energy value $E \in \mathbb{R}$ and some $\varepsilon > 0$ such that $H_{0,s}^{-1}([E-\varepsilon, E+\varepsilon]) \subset \mathbb{R}^d \times \mathbb{R}^d$ is compact.
3. $H_{0,s}$ has no critical value in $[E-\varepsilon, E+\varepsilon]$.
4. $(H_{0,s} + \mathrm{i})$ is elliptic in the sense that

   $$|H_{0,s}(\boldsymbol{p}, \boldsymbol{x}) + \mathrm{i}| \geq C \, m(\boldsymbol{p}, \boldsymbol{x}) \ , \tag{2.16}$$

   with some $C > 0$.

If $\hbar$ is small enough, the above properties of $H_{0,s}$ ensure that the spectrum of $\hat{H}$ is purely discrete in any interval which is properly contained in $[E-\varepsilon, E+\varepsilon]$, and that $\hat{H}$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^d) \otimes \mathbb{C}^n$. For simplicity, we denote the self-adjoint extensions, which are the relevant quantum mechanical Hamiltonians, also by $\hat{H}$. Furthermore, if $f \in C_0^\infty(\mathbb{R})$, the operator $f(\hat{H})$ defined by the functional calculus given by the spectral theorem is a

Weyl operator with symbol $\phi \in \mathrm{S}^0(m^{-r})$ for every $r \in \mathbb{R}$. Its asymptotic expansion is given by

$$\phi \sim \sum_{j=0}^{\infty} \hbar^j \phi_j \ , \tag{2.17}$$

with $\phi_0(\boldsymbol{p},\boldsymbol{x}) = f(H_{0,s}(\boldsymbol{p},\boldsymbol{x}))\mathbb{1}_n$ and $\phi_1(\boldsymbol{p},\boldsymbol{x}) = H_1(\boldsymbol{p},\boldsymbol{x}) f'(H_{0,s}(\boldsymbol{p},\boldsymbol{x}))$. The above properties are proven in [Rob87, DS99] for the case of scalar valued symbols. These proofs can immediately be carried over to the present situation in which the principal symbol H_0 of the Hamiltonian is a scalar multiple of $\mathbb{1}_n$.

We remark that the requirement $H_0 \in \mathrm{S}(m)$ together with (2.16) implies that

$$C^2\, m^2(\boldsymbol{p},\boldsymbol{x}) \leq 1 + H_{0,s}^2(\boldsymbol{p},\boldsymbol{x}) \leq D^2\, m^2(\boldsymbol{p},\boldsymbol{x}) + 1 \ , \tag{2.18}$$

so that $(1+H_{0,s}^2)^{1/2}$ is an order function. Moreover, the condition $H_j \in \mathrm{S}(m)$ is equivalent to $H_j \in \mathrm{S}((1+H_{0,s}^2)^{1/2})$, which is the requirement on the symbol imposed in [Rob87, HMR87].

Below we will study the semiclassical behaviour of quantum mechanical observables and of their expectation values in eigenstates of the Hamiltonian. For these purposes it will be advantageous to restrict attention to bounded observables. In order to characterise a sufficiently large class of such operators we employ

Proposition 2.3 (Calderón-Vaillancourt). *Let $B \in \mathrm{S}^0(1)$, then the Weyl quantised operator $\hat{B}$ is bounded on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$. Moreover, for $\hbar \in (0,1]$ there exists an upper bound for the operator norms of $\hat{B}$.*

The original version of this Proposition goes back to Calderón and Vaillancourt [CV71]. In the form presented here, it can be found (for scalar valued symbols) in [DS99]; that proof can be directly carried over to the present situation. Furthermore, if we require the symbols $B \in \mathrm{S}^0(1)$ to be hermitian matrices, their Weyl quantisations $\hat{B}$ are symmetric operators that can be extended to self-adjoint operators on all of $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$; the latter we also denote by $\hat{B}$. The above properties can immediately be generalised to the case $B \in \mathrm{S}^k(1)$. Then, however, one has to extract a factor of $\hbar^{-k}$ from the norm of $\hat{B}$ in order to obtain the bound on the norms when $\hbar$ varies in $(0,1]$.

3 Semiclassical time evolution and Szegö limit formula

The quantum mechanical time evolution as, e.g., governed by the Pauli equation (2.1) requires to investigate the Cauchy problem for the operator

$$\mathrm{i}\hbar \frac{\partial}{\partial t} - \hat{H} \tag{3.1}$$

on $L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$. This problem can be solved by introducing the one-parameter group of unitary operators

$$\hat{U}(t) := \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t} , \tag{3.2}$$

which are well defined for all $t \in \mathbb{R}$ since $\hat{H}$ is (essentially) self-adjoint. The time evolution of a quantum mechanical observable $\hat{B}$, which arises as the Weyl quantisation of a symbol $B \in \mathrm{S}^k_{\mathrm{cl}}(1)$, is then given by

$$\hat{B}(t) := \hat{U}^\dagger(t)\, \hat{B}\, \hat{U}(t) . \tag{3.3}$$

The time-evolved observable (3.3) therefore satisfies the Heisenberg equation of motion

$$\frac{\partial}{\partial t}\hat{B}(t) = \frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{B}(t)] , \qquad \hat{B}(0) = \hat{B} . \tag{3.4}$$

For Weyl operators $\hat{H}$ and $\hat{B}$ with scalar symbols it is well known that for finite times t the propagators $\hat{U}(t)$ are semiclassical Fourier integral operators which arise as quantisations of the Hamiltonian flow generated by the principal symbol $H_{0,s}$ of the quantum Hamiltonian $\hat{H}$. In addition, the time evolution (3.3) respects operator classes in the sense that if $\hat{B}$ is a quantisation of a symbol in some suitable class such as $\mathrm{S}^k_{\mathrm{cl}}(1)$, $\hat{B}(t)$ is again an operator with symbol in the same class (see, e.g., [Rob87]).

In the case of matrix valued symbols the situation is different; in physical terms this has to do with the need to propagate the internal (i.e. spin) degrees of freedom in addition to the translational ones. To begin with, let us hence introduce the Hamiltonian vector field $X_{H_{0,s}} := (-\partial_x H_{0,s}, \partial_p H_{0,s})$ associated with the scalar factor $H_{0,s}$ of the principal symbol H_0, and denote by Φ^t the flow generated by $X_{H_{0,s}}$. That is, $(\boldsymbol{p}(t), \boldsymbol{x}(t)) = \Phi^t(\boldsymbol{p}, \boldsymbol{x})$ is a solution of Hamilton's equations of motion

$$\dot{\boldsymbol{p}}(t) = -\partial_x H_{0,s}(\boldsymbol{p}(t), \boldsymbol{x}(t)) , \qquad \dot{\boldsymbol{x}}(t) = \partial_p H_{0,s}(\boldsymbol{p}(t), \boldsymbol{x}(t)) , \tag{3.5}$$

with initial condition $(\boldsymbol{p}(0), \boldsymbol{x}(0)) = (\boldsymbol{p}, \boldsymbol{x})$. This describes the classical dynamics of the translational degrees of freedom, whereas the propagation of the spin degrees of freedom is only contained in the dynamics of the (matrix valued) symbol $B(t)$. For the following we suppose that $\hat{B}$ is a Weyl operator with symbol $B \in \mathrm{S}^k_{\mathrm{cl}}(1)$. Then (3.3) yields the observable $\hat{B}(t)$, which is a Weyl quantisation of some symbol $B(t)$ that in general will not be in the class $\mathrm{S}^k_{\mathrm{cl}}(1)$, although, however, $\hat{B}(t)$ clearly remains a bounded operator. We hence base the following construction on the formal asymptotic expansion

$$B(t) \sim \sum_{l=0}^{\infty} \hbar^{-k+l}\, B_l(t) , \tag{3.6}$$

whose coefficients can be determined from the Heisenberg equations of motion (3.4), once these have been transfered to the level of symbols with the help of the product formula

(2.14); the latter also applies to operators with symbols that have a formal asymptotic expansion of the type (3.6). We thus obtain the recursive Cauchy problem,

$$\frac{\partial}{\partial t} B_l(t) - \{H_0, B_l(t)\} - \mathrm{i}\,[H_1, B_l(t)] = \sum_{\substack{0\leq k\leq l-1 \\ j+|\alpha|+|\beta|=l-k}} \frac{\mathrm{i}^{|\alpha|-|\beta|}}{2^{|\alpha|+|\beta|}|\alpha|!|\beta|!} \Big(\big(\partial_p^\beta \partial_x^\alpha B_k(t)\big)\big(\partial_p^\alpha \partial_x^\beta H_j\big) - (-1)^{|\alpha|-|\beta|}\big(\partial_p^\alpha \partial_x^\beta H_j\big)\big(\partial_p^\beta \partial_x^\alpha B_k(t)\big)\Big) , \tag{3.7}$$

with $B_l(0) = B_l$, compare [Ivr98, ch.2.3]. Here

$$\{A, B\} := \partial_p A \cdot \partial_x B - \partial_x A \cdot \partial_p B \tag{3.8}$$

denotes the Poisson bracket of $A, B \in C^\infty(\mathbb{R}^d \times \mathbb{R}^d) \otimes \mathbb{C}^{n\times n}$; notice that in general $\{A, B\} \neq -\{B, A\}$. In leading semiclassical order (3.7) now yields the following equation for the principal symbol $B_0(t)$,

$$\frac{\partial}{\partial t} B_0(t) - \{H_0, B_0(t)\} - \mathrm{i}\,[H_1, B_0(t)] = 0 , \tag{3.9}$$

which for Hamiltonians with a scalar sub-principal symbol H_1 reduces to

$$\frac{\partial}{\partial t} B_0(t) - \{H_0, B_0(t)\} = \frac{\mathrm{d}}{\mathrm{d}t}\left(B_0(t) \circ \Phi^{-t}\right) = 0 . \tag{3.10}$$

In order to solve the general case, (3.9) is rewritten as

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[d^{-1}(\boldsymbol{p}, \boldsymbol{x}, -t)\, B_0(t)(\Phi^{-t}(\boldsymbol{p}, \boldsymbol{x}))\, d(\boldsymbol{p}, \boldsymbol{x}, -t)\right] = 0 , \tag{3.11}$$

where d has to fulfill

$$\dot{d}(\boldsymbol{p}, \boldsymbol{x}, t) + \mathrm{i}\, H_1(\Phi^t(\boldsymbol{p}, \boldsymbol{x}))\, d(\boldsymbol{p}, \boldsymbol{x}, t) = 0 , \qquad d(\boldsymbol{p}, \boldsymbol{x}, 0) = \mathbb{1}_n . \tag{3.12}$$

Here the time derivative has to be understood along the trajectory $\Phi^t(\boldsymbol{p}, \boldsymbol{x})$. The quantity d already appeared in [BK99a, BK99b], where it was introduced in order to describe the (semiclassical) propagation of the spin degrees of freedom along the trajectories of the Hamiltonian flow Φ^t.

We are now in a position to calculate the principal symbol of $\hat{B}(t)$ from (3.11),

$$B_0(t)(\boldsymbol{p}, \boldsymbol{x}) = d(\Phi^t(\boldsymbol{p}, \boldsymbol{x}), -t)\, B_0(\Phi^t(\boldsymbol{p}, \boldsymbol{x}))\, d^{-1}(\Phi^t(\boldsymbol{p}, \boldsymbol{x}), -t) . \tag{3.13}$$

Equivalently, employing the property

$$d(\Phi^t(\boldsymbol{p}, \boldsymbol{x}), -t) = d^{-1}(\boldsymbol{p}, \boldsymbol{x}, t) \tag{3.14}$$

that can be deduced from (3.12) (see, e.g., [BN99]) one obtains

$$B_0(t)(\boldsymbol{p},\boldsymbol{x}) = d^{-1}(\boldsymbol{p},\boldsymbol{x},t)\, B_0(\Phi^t(\boldsymbol{p},\boldsymbol{x}))\, d(\boldsymbol{p},\boldsymbol{x},t)\ . \tag{3.15}$$

Notice that in [BN99] the quantity $\Gamma(t,\boldsymbol{p},\boldsymbol{x}) = d^{-1}(\boldsymbol{p},\boldsymbol{x},t)$ is used instead of $d(\boldsymbol{p},\boldsymbol{x},t)$. If we take into account that $d(\boldsymbol{p},\boldsymbol{x},t)$ is unitary, which follows from (3.12) since H_1 is hermitian (see, e.g., [BK99a, BN99]), then (3.15) also reads

$$B_0(t)(\boldsymbol{p},\boldsymbol{x}) = d^{\dagger}(\boldsymbol{p},\boldsymbol{x},t)\, B_0(\Phi^t(\boldsymbol{p},\boldsymbol{x}))\, d(\boldsymbol{p},\boldsymbol{x},t)\ , \tag{3.16}$$

which is the form that we will use below.

In principle one could determine all coefficients $B_l(t)$ in this fashion, but one must be aware of the fact that the resulting symbol $B(t)$ will in general not be in $\mathrm{S}^k_{\mathrm{cl}}(1)$, unless one restricts the growth of the symbol H in such a way that one would exclude the Pauli Hamiltonians (2.2) that we are interested in. If, however, one restricts attention to observables whose symbols have compact support, $B \in C_0^\infty(\mathbb{R}^d \times \mathbb{R}^d) \otimes \mathbb{C}^{n\times n}$, this problem is avoided and one obtains a Weyl symbol $B_{sum}(t) \in C_0^\infty(\mathbb{R}^d \times \mathbb{R}^d) \otimes \mathbb{C}^{n\times n}$ by, say, Borel summation of the asymptotic expansion (3.6), with the solutions $B_l(t)$ of the recursive Cauchy problem (3.7) entering. On the level of the corresponding operators one therefore finds

$$\left\| \widehat{B_{sum}(t)} - \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\, \hat{B}\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t} \right\|_{\mathcal{L}} \leq C\,\hbar^N\ , \qquad \text{for all } N \in \mathbb{N}\ , \tag{3.17}$$

where $\|\cdot\|_{\mathcal{L}}$ denotes the norm on $\mathcal{L}(L^2(\mathbb{R}^d)\otimes\mathbb{C}^n, L^2(\mathbb{R}^d)\otimes\mathbb{C}^n)$.

The same result, which is a variant of the Egorov Theorem [Ego69], can be achieved for general $B \in \mathrm{S}^k_{\mathrm{cl}}(1)$ under suitable requirements on the symbol of the Hamiltonian $\hat{H}$ (see [Ivr98, ch.2.3]):

Proposition 3.1. *Let H be in $\mathrm{S}(m)$ and $B \in \mathrm{S}^k_{\mathrm{cl}}(1)$ and suppose that*

$$\left\|\partial_p^\alpha \partial_x^\beta H_j(\boldsymbol{p},\boldsymbol{x})\right\| \leq C \quad \textit{for all} \quad (\boldsymbol{p},\boldsymbol{x}) \in \mathbb{R}^d \times \mathbb{R}^d \quad \textit{and} \quad |\alpha| + |\beta| + 2j \geq 2\ . \tag{3.18}$$

Then the estimate

$$\left\| \widehat{B_{sum}(t)} - e^{\frac{i}{\hbar}\hat{H}t}\, \hat{B}\, e^{-\frac{i}{\hbar}\hat{H}t} \right\|_{\mathcal{L}} \leq D\,\hbar^N \tag{3.19}$$

holds for arbitrary $N > 0$ and $t \in [0,T]$.

Let us remark that under the assumption (3.18) the Hamiltonian vector field $X_{H_{0,s}}$ grows at most linearly at infinity. Therefore, a trajectory $\Phi^t(\boldsymbol{p},\boldsymbol{x})$ cannot blow up at finite times so that the flow exists globally on $\mathbb{R}^d\times\mathbb{R}^d$ (see, e.g., [Rob87]). We have not made any attempt at improving the bounds on the time T, in terms of $\hbar$, up to which Proposition 3.1 holds, since for our further purposes we are mainly interested in the relation (3.16). For the scalar case such improvements have, however, been established in [BGP99, BR99].

As a second essential input for the proof of quantum ergodicity, in addition to the Egorov property (3.16), we require a Szegö limit formula (see, e.g., [Gui79]) that connects averaged expectation values of an observable semiclassically with a classical average. On the quantum mechanical side we consider an interval $I(E,\hbar) := [E-\hbar\omega, E+\hbar\omega]$, with some $\omega > 0$, such that $I(E,\hbar) \subseteq [E-\varepsilon, E+\varepsilon]$ if $\hbar$ is sufficiently small. According to the assumptions 1.–4. on the Hamiltonian $\hat{H}$ in section 2 the spectrum of $\hat{H}$ in $I(E,\hbar)$ is therefore discrete. We then denote the number of eigenvalues contained in $I(E,\hbar)$ by N_I, and $\{\psi_k\}$ shall be the (orthonormal) eigenvectors of $\hat{H}$ associated with the eigenvalues $E_k \in I(E,\hbar)$. On the classical side, let $\Omega_E := H_{0,s}^{-1}(E)$ be the hypersurface of energy E in phase space and denote the normalised Liouville measure on Ω_E by $\mathrm{d}\mu_E$, i.e.

$$\mathrm{d}\mu_E(\boldsymbol{p},\boldsymbol{x}) = \frac{1}{\mathrm{vol}\,\Omega_E}\,\delta\big(H_{0,s}(\boldsymbol{p},\boldsymbol{x}) - E\big)\;\mathrm{d}p\,\mathrm{d}x\ . \tag{3.20}$$

In the following we will abbreviate averages of (smooth) matrix valued functions $B \in C^\infty(\mathbb{R}^d \times \mathbb{R}^d) \otimes \mathbb{C}^{n\times n}$ over Ω_E by

$$\mu_E(B) := \int_{\Omega_E} B(\boldsymbol{p},\boldsymbol{x})\;\mathrm{d}\mu_E(\boldsymbol{p},\boldsymbol{x})\ . \tag{3.21}$$

From now on we also suppose that the Hamiltonian flow Φ^t generated by $H_{0,s}$ is ergodic with respect to μ_E, i.e. for $f \in L^1(\Omega_E, d\mu_E)$ and μ_E-almost all $(\boldsymbol{p},\boldsymbol{x}) \in \Omega_E$

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T f\big(\Phi^t(\boldsymbol{p},\boldsymbol{x})\big)\;\mathrm{d}t = \int_{\Omega_E} f(\boldsymbol{q},\boldsymbol{y})\;\mathrm{d}\mu_E(\boldsymbol{q},\boldsymbol{y})\ . \tag{3.22}$$

This in particular implies that the set of periodic points of Φ^t with periods $T > 0$ has Liouville measure zero.

The rest of this section will now be devoted to the proof of

Proposition 3.2 (Szegö limit formula). *Let $\hat{H}$ be a quantum Hamiltonian with symbol $H \in \mathrm{S}^0_{\mathrm{cl}}(m)$, where $m \geq 1$, that fulfills the properties 1.–4. of section 2. If then $\hat{B}$ is an observable with symbol $B \in \mathrm{S}^0_{\mathrm{cl}}(1)$ and principal symbol B_0, the following Szegö limit formula holds,*

$$\lim_{\hbar\to 0}\frac{1}{N_I}\sum_{E_k\in I(E,\hbar)}\langle\psi_k, \hat{B}\psi_k\rangle = \frac{1}{n}\,\mathrm{tr}\,\mu_E(B_0)\ . \tag{3.23}$$

Proof. In principle we adopt the method presented in [DS99], and modify it appropriately where necessary. Let us first recall that if $g \in C_0^\infty(\mathbb{R})$ is suitably chosen, with $g(\lambda) = \lambda$ on a neighbourhood of the interval $I(E,\hbar)$, the operator $g(\hat{H})$ has the same spectrum in $I(E,\hbar)$ as $\hat{H}$ itself. Furthermore, the symbol $H_g \in \mathrm{S}^0_{\mathrm{cl}}(1)$ of $g(\hat{H})$ has an asymptotic expansion that coincides on $H_{0,s}^{-1}(I(E,\hbar))$ with that of H. Since below we are localising in energy to the interval $I(E,\hbar)$ so that we can consider $g(\hat{H})$ instead of $\hat{H}$, from now on we simply suppose that $H \in \mathrm{S}^0_{\mathrm{cl}}(1)$.

Let now $\chi \in C_0^\infty(\mathbb{R})$ be given with $\chi \equiv 1$ on $I(E,\hbar)$ and such that the spectrum of $\hat{H}$ in supp χ is discrete. This might require to choose $\hbar$ small enough. Then consider the (energy localised) quantum mechanical time evolution operator

$$\hat{U}_\chi(t) := \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}\,\chi(\hat{H}) \; . \tag{3.24}$$

Up to an error of order $O(\hbar^\infty)$ in trace norm, this operator can be approximated by a semiclassical Fourier integral operator with kernel

$$K_\chi(\boldsymbol{x},\boldsymbol{y},t) = \frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^d} a_\hbar(\boldsymbol{x},\boldsymbol{y},t,\boldsymbol{\xi})\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S(\boldsymbol{x},\boldsymbol{\xi},t)-\boldsymbol{\xi}\cdot\boldsymbol{y})}\,\mathrm{d}\xi \; , \tag{3.25}$$

if $|t|$ is small enough (see, e.g., [DS99]). We remark that here the amplitude $a_\hbar$ takes values in $\mathbb{C}^{n\times n}$, thus it also represents the internal (i.e. spin) degrees of freedom. As explained in [BK99a], the phase S in (3.25) is then given as the solution of the Hamilton-Jacobi equation

$$H_{0,s}\big(\partial_x S(\boldsymbol{x},\boldsymbol{\xi},t),\boldsymbol{x}\big) + \partial_t S(\boldsymbol{x},\boldsymbol{\xi},t) = 0 \; , \qquad S(\boldsymbol{x},\boldsymbol{\xi},0) = \boldsymbol{x}\cdot\boldsymbol{\xi} \; . \tag{3.26}$$

In leading semiclassical order the transport equation for $a_\hbar \sim a_0 + \hbar\, a_1 + \dots$ can be solved by a separation of the internal degrees of freedom from the translational ones. The latter lead to the expression known from the scalar case (see, e.g., [DS99]), whereas the modifications required by the matrix character of a_0 are provided by the solution $d(\boldsymbol{p},\boldsymbol{x},t)$ of (3.12), see [BK99a]. For the present purpose, however, one only needs the initial condition $a_\hbar|_{t=0} = \chi(H_{0,s})\mathbb{1}_n + O(\hbar)$.

In a next step we consider $\rho \in C^\infty(\mathbb{R})$ with Fourier transform $\tilde{\rho} \in C_0^\infty(\mathbb{R})$ such that

$$\mathrm{Tr}\,\frac{1}{2\pi}\int_{\mathbb{R}} \tilde{\rho}(t)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}Et}\,\hat{B}\,\hat{U}_\chi(t)\;\mathrm{d}t = \sum_k \chi(E_k)\,\langle\psi_k,\hat{B}\psi_k\rangle\,\rho\left(\frac{E_k-E}{\hbar}\right) \; , \tag{3.27}$$

where $\mathrm{Tr}\,(\cdot)$ denotes the operator trace on $L^2(\mathbb{R}^d)\otimes\mathbb{C}^n$. Approximating $\hat{U}_\chi(t)$ with the help of (3.25), in leading semiclassical order one then has to calculate

$$\frac{1}{2\pi\,(2\pi\hbar)^d}\int_{\mathbb{R}}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \tilde{\rho}(t)\;\mathrm{tr}\big(B_0(\partial_x S,\boldsymbol{x})\,a_0(\boldsymbol{x},\boldsymbol{x},t,\boldsymbol{\xi})\big)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S(\boldsymbol{x},\boldsymbol{\xi},t)-\boldsymbol{\xi}\cdot\boldsymbol{x}+Et)}\,\mathrm{d}\xi\,\mathrm{d}x\,\mathrm{d}t \tag{3.28}$$

with the method of stationary phase. The stationary points of the phase $S(\boldsymbol{x},\boldsymbol{\xi},t)-\boldsymbol{\xi}\cdot\boldsymbol{x}+Et$ are given by $(\boldsymbol{\xi}_{st},\boldsymbol{x}_{st},t_{st}) \in \mathbb{R}^d\times\mathbb{R}^d\times\mathbb{R}$ such that $(\boldsymbol{\xi}_{st},\boldsymbol{x}_{st}) \in \Omega_E$ is a periodic point of the Hamiltonian flow Φ^t with period t_{st}. Since we have assumed that E is not a critical value for $H_{0,s}$, the periods of Φ^t on Ω_E do not accumulate at zero, see [Rob87]. Hence, if the support of $\tilde{\rho}$ is chosen small enough, the manifold of critical points contributing to (3.28) is given by $\Omega_E\times\{0\}$. In analogy to [BK99a] we thus obtain

$$\sum_k \chi(E_k)\,\langle\psi_k,\hat{B}\psi_k\rangle\,\rho\left(\frac{E_k-E}{\hbar}\right) = \chi(E)\,\frac{\tilde{\rho}(0)}{2\pi}\,\frac{\mathrm{vol}\,\Omega_E}{(2\pi\hbar)^{d-1}}\,\big(\mathrm{tr}\,\mu_E(B_0)+O(\hbar)\big) \; . \tag{3.29}$$

Moreover, since we require $H_{0,s}$ to be such that no $E' \in [E-\varepsilon, E+\varepsilon]$ is a critical value and all $\Omega_{E'}$ are compact, (3.29) holds true with E replaced by E' uniformly in $[E-\varepsilon, E+\varepsilon]$. In a last step we now apply the Tauberian Lemma of [BPU95], which takes non-negative weights into account. To this end we have to ensure that $\langle \psi_k, \hat{B}\psi_k \rangle$ is non-negative. However, since $\hat{B}$ is bounded, this can always be achieved by adding a suitable constant. Moreover, according to our above choice of χ we find that $\chi(E) = 1$ and $\chi(E_k) = 1$ for all $E_k \in I(E, \hbar)$. Therefore

$$\sum_{E_k \in I(E,\hbar)} \langle \psi_k, \hat{B}\psi_k \rangle = \frac{\omega}{\pi} \frac{\operatorname{vol}\Omega_E}{(2\pi\hbar)^{d-1}} \operatorname{tr} \mu_E(B_0) + o(\hbar^{1-d}) \ . \tag{3.30}$$

Repeating the above reasoning with the identity instead of $\hat{B}$, one can express the number N_I of eigenvalues in $I(E, \hbar)$ semiclassically,

$$N_I = \frac{n\omega}{\pi} \frac{\operatorname{vol}\Omega_E}{(2\pi\hbar)^{d-1}} + o(\hbar^{1-d}) \ . \tag{3.31}$$

Thus, (3.30) and (3.31) together finally yield the Szegö limit formula (3.23). □

4 Quantum ergodicity

In the following we will restrict attention to the case of spin $s = 1/2$, which is both the simplest and physically most important situation. This means that below $n = 2s + 1 = 2$ will be chosen, so that all symbols of observables and Hamiltonians take values in the hermitian 2×2 matrices. We also assume that the quantum Hamiltonian describes the coupling of translational and spin degrees of freedom as in (2.2). This restricts the subprincipal symbol H_1 of $\hat{H}$ to be a traceless hermitian matrix. As a consequence, the spin transport equation (3.12) is solved by a spin transport matrix $d(\boldsymbol{p}, \boldsymbol{x}, t) \in \mathrm{SU}(2)$.

Our strategy of approaching quantum ergodicity is inspired by the method introduced in [Zel96, ZZ96], which does not require to rely on a positive quantisation, such as anti-Wick or Friedrichs quantisation. It is rather based on an analysis of the expression

$$S_2(E, \hbar) := \frac{1}{N_I} \sum_{E_k \in I(E,\hbar)} \left| \langle \psi_k, \hat{B}\psi_k \rangle - \frac{1}{2} \operatorname{tr} \mu_E(B_0) \right|^2 , \tag{4.1}$$

which is the variance of the expectation values of the quantum observable $\hat{B}$ about the classical mean value of its principal symbol B_0. We are in particular interested in the behaviour of (4.1) in the limit $\hbar \to 0$. For this purpose we introduce the bounded and self-adjoint auxiliary operator

$$\hat{B}_T := \frac{1}{T} \int_0^T \hat{U}^\dagger(t)\, \hat{B}\, \hat{U}(t)\ \mathrm{d}t - \frac{1}{2} \operatorname{tr} \mu_E(B_0)\, \mathbb{1}_2 \ . \tag{4.2}$$

Its expectation values in eigenstates of the Hamiltonian are

$$\langle\psi_k, \hat{B}_T\psi_k\rangle = \langle\psi_k, \hat{B}\psi_k\rangle - \frac{1}{2}\operatorname{tr}\mu_E(B_0)\ , \tag{4.3}$$

such that

$$S_2(E,\hbar) = \frac{1}{N_I}\sum_{E_k\in I(E,\hbar)} \left|\langle\psi_k, \hat{B}_T\psi_k\rangle\right|^2 . \tag{4.4}$$

Using the Egorov property (3.16), the principal symbol of the auxiliary operator reads

$$B_{T,0}(\boldsymbol{p},\boldsymbol{x}) = \frac{1}{T}\int_0^T d^\dagger(\boldsymbol{p},\boldsymbol{x},t)\, B_0(\Phi^t(\boldsymbol{p},\boldsymbol{x}))\, d(\boldsymbol{p},\boldsymbol{x},t)\ \mathrm{d}t - \frac{1}{2}\operatorname{tr}\mu_E(B_0)\,\mathbb{1}_2\ . \tag{4.5}$$

Comparing this expression with the analogous one obtained in the scalar case, one observes that the principal symbol B_0 is not only transported by the flow Φ^t, but also conjugated with the spin transport matrix $d(\boldsymbol{p},\boldsymbol{x},t)$. Thus both the translational and the spin dynamics are involved. This observation suggests that the ergodicity of the flow Φ^t will no longer suffice to yield quantum ergodicity. One therefore has to combine the classical dynamics of the translational degrees of freedom and the spin dynamics in a suitable way, and then one demands ergodic properties of the combined dynamics. In order to achieve this we employ the same construction as in [BK99b] and hence introduce the product phase space

$$\mathcal{M} := \Omega_E \times \mathrm{SU}(2)\ . \tag{4.6}$$

The combined flow $Y^t : \mathcal{M}\to\mathcal{M}$ is then defined as an SU(2)-extension of the Hamiltonian flow Φ^t on Ω_E, i.e. for $(\boldsymbol{p},\boldsymbol{x})\in\Omega_E$ and $g\in\mathrm{SU}(2)$ we set

$$Y^t((\boldsymbol{p},\boldsymbol{x}),g) := \big(\Phi^t(\boldsymbol{p},\boldsymbol{x}), d(\boldsymbol{p},\boldsymbol{x},t)g\big)\ . \tag{4.7}$$

The initial condition $Y^0 = \mathrm{id}$ is obviously fulfilled, and $Y^{t+s} = Y^t\circ Y^s$ follows from the composition law

$$d(\boldsymbol{p},\boldsymbol{x},t+s) = d\big(\Phi^t(\boldsymbol{p},\boldsymbol{x}),s\big)\, d(\boldsymbol{p},\boldsymbol{x},t) \tag{4.8}$$

that derives from the spin transport equation (3.12). In ergodic theory such a combined dynamics is also known as a skew product (see, e.g., [CFS82]). On $\mathcal{M}$ the product measure $\mu := \mu_E\times\mu_H$ consisting of the Liouville measure μ_E on Ω_E and the normalised Haar measure μ_H on SU(2) is introduced. This measure is normalised and invariant under the flow Y^t, since μ_E is normalised and invariant under Φ^t and μ_H is both left and right invariant. Ergodicity of Y^t on $\mathcal{M}$ with respect to μ then means that for $F\in L^1(\mathcal{M},\mathrm{d}\mu)$

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T F\big(Y^t((\boldsymbol{p},\boldsymbol{x}),g)\big)\ \mathrm{d}t = \int_{\mathcal{M}} F((\boldsymbol{q},\boldsymbol{y}),h)\ \mathrm{d}\mu((\boldsymbol{q},\boldsymbol{y}),h) \tag{4.9}$$

holds for μ-almost all $((\boldsymbol{p},\boldsymbol{x}),g)\in\mathcal{M}$. In particular, if one chooses F to be independent of g, then (4.9) reduces to the condition (3.22), so that the ergodicity of the extended flow Y^t on $\mathcal{M}$ implies the ergodicity of the flow Φ^t on the base manifold Ω_E.

Our main result now states the effect of the ergodicity of Y^t on the semiclassical asymptotics of eigenfunctions of $\hat{H}$.

Theorem 4.1 (Quantum ergodicity). *Let $\hat{H}$ be a quantum Hamiltonian with symbol $H \in \mathrm{S}^0_{\mathrm{cl}}(m)$, where $m \geq 1$, and principal symbol $H_0 = H_{0,s}\mathbb{1}_2$, which fulfills the conditions 1.–4. of section 2 and, furthermore, satisfies*

$$\|\partial_p^\alpha \partial_x^\beta H_j(\boldsymbol{p},\boldsymbol{x})\| \leq C \quad \text{for all} \quad (\boldsymbol{p},\boldsymbol{x}) \in \mathbb{R}^d \times \mathbb{R}^d \quad \text{and} \quad |\alpha|+|\beta|+2j \geq 2. \tag{3.18}$$

Then, under the condition that Y^t is ergodic on $\mathcal{M}$ with respect to μ, in every sequence $\{\psi_k \mid E_k \in I(E,\hbar)\}$ of orthonormal eigenfunctions of $\hat{H}$ there exists a subsequence $\{\psi_{k_j} \mid E_{k_j} \in I(E,\hbar)\}$ of density one, i.e.

$$\lim_{\hbar\to 0} \frac{\#\{j \mid E_{k_j} \in I(E,\hbar)\}}{\#\{k \mid E_k \in I(E,\hbar)\}} = 1 \ , \tag{4.10}$$

such that for every quantum observable $\hat{B}$ with hermitian symbol $B \in \mathrm{S}^0_{\mathrm{cl}}(1)$ and principal symbol B_0

$$\lim_{j\to\infty} \langle \psi_{k_j}, \hat{B}\psi_{k_j}\rangle = \frac{1}{2}\,\mathrm{tr}\,\mu_E(B_0) \ . \tag{4.11}$$

Moreover, the subsequence $\{\psi_{k_j}\}$ can be chosen independent of the observable $\hat{B}$.

Proof. An application of the Cauchy-Schwartz inequality on the right-hand side of (4.4) yields an upper bound for the quantity (4.1) that reads

$$S_2(E,\hbar) \leq \frac{1}{N_I} \sum_{E_k \in I(E,\hbar)} \langle \psi_k, (\hat{B}_T)^2 \psi_k\rangle \ . \tag{4.12}$$

In order to determine the limit as $\hbar \to 0$ of (4.12) one can now apply Proposition 3.2, which gives

$$\lim_{\hbar\to 0} S_2(E,\hbar) \leq \frac{1}{2}\,\mathrm{tr}\,\mu_E\big((B_{T,0})^2\big) \ . \tag{4.13}$$

Quantum ergodicity then follows, if the bound on the right-hand side can be shown to vanish. This will indeed be possible in the limit $T \to \infty$. In order to achieve this we first employ the ergodicity of Y^t in that we choose $F((\boldsymbol{q},\boldsymbol{y}),h) = h^\dagger\, B_0(\boldsymbol{q},\boldsymbol{y})\, h$ in the relation (4.9), and thus find

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T g^\dagger\, d^\dagger(\boldsymbol{p},\boldsymbol{x},t)\, B_0(\Phi^t(\boldsymbol{p},\boldsymbol{x}))\, d(\boldsymbol{p},\boldsymbol{x},t)\, g \ \mathrm{d}t = \int_{\mathrm{SU}(2)} h^\dagger\, \mu_E(B_0)\, h \ \mathrm{d}\mu_H(h) \tag{4.14}$$

for μ_E-almost all $(\boldsymbol{p},\boldsymbol{x}) \in \Omega_E$ and μ_H-almost all $g \in \mathrm{SU}(2)$. In terms of the principal symbol (4.5) of the auxiliary operator $\hat{B}_T$ this means

$$\lim_{T\to\infty} g^\dagger\, B_{T,0}(\boldsymbol{p},\boldsymbol{x})\, g = \int_{\mathrm{SU}(2)} h^\dagger\, \mu_E(B_0)\, h \ \mathrm{d}\mu_H(h) - \frac{1}{2}\,\mathrm{tr}\,\mu_E(B_0)\,\mathbb{1}_2 \ . \tag{4.15}$$

Our next goal is to calculate the right-hand side of (4.15). To this end we represent the hermitian 2×2 matrix $\mu_E(B_0)$ as a linear combination of $\mathbb{1}_2$ and the Pauli matrices σ_k, i.e. $\mu_E(B_0) = \frac{1}{2}\operatorname{tr}\mu_E(B_0) + \boldsymbol{b}\cdot\boldsymbol{\sigma}$, where $\boldsymbol{b}\in\mathbb{R}^3$. We then recall that for every $g\in\mathrm{SU}(2)$ the adjoint map $\mathrm{Ad}_g : \mathrm{su}(2)\to\mathrm{su}(2)$ is defined as $\mathrm{Ad}_g(X) = g^\dagger X\, g$. Thus, $\mathrm{Ad}_h(\boldsymbol{b}\cdot\boldsymbol{\sigma})\in\mathrm{su}(2)$ can be expanded in terms of the Pauli matrices σ_k such that $h^\dagger\,\boldsymbol{b}\cdot\boldsymbol{\sigma}\,h = (\varphi(h)\boldsymbol{b})\cdot\boldsymbol{\sigma}$. The map $\varphi:\ \mathrm{SU}(2)\to\mathrm{SO}(3)$ that results in this way can be identified as the universal (twofold) covering of SO(3) by SU(2). Therefore

$$\int_{\mathrm{SU}(2)} h^\dagger\,\mu_E(B_0)\,h\ \mathrm{d}\mu_H(h) = \frac{1}{2}\operatorname{tr}\mu_E(B_0)\,\mathbb{1}_2 + \left(\int_{\mathrm{SU}(2)}\varphi(h)\ \mathrm{d}\mu_H(h)\,\boldsymbol{b}\right)\cdot\boldsymbol{\sigma}\ . \tag{4.16}$$

We now show that the second term on the right-hand side of (4.16) vanishes. To this end we multiply the integral over SU(2), which yields a 3×3 matrix, with an arbitrary orthogonal matrix $R\in\mathrm{SO}(3)$ from the left. We then exploit the fact that there exists $\tilde g\in\mathrm{SU}(2)$ such that $R=\varphi(\tilde g)$, together with the left invariance of the Haar measure, in order to conclude that

$$R\int_{\mathrm{SU}(2)}\varphi(h)\ \mathrm{d}\mu_H(h) = \int_{\mathrm{SU}(2)}\varphi(\tilde g h)\ \mathrm{d}\mu_H(h) = \int_{\mathrm{SU}(2)}\varphi(h)\ \mathrm{d}\mu_H(h)\ . \tag{4.17}$$

Since hence the 3×3 matrix represented by the integral over SU(2) is invariant under left multiplication by an arbitrary element of SO(3), it must be the zero matrix. Therefore, the right-hand side of (4.15) vanishes.

We now choose some $g\in\mathrm{SU}(2)$ such that (4.14) holds and therefore obtain that

$$\lim_{T\to\infty}\operatorname{tr}\bigl(B_{T,0}(\boldsymbol{p},\boldsymbol{x})\bigr)^2 = \lim_{T\to\infty}\operatorname{tr}\bigl(g^\dagger\,B_{T,0}(\boldsymbol{p},\boldsymbol{x})\,g\bigr)^2 = 0 \tag{4.18}$$

holds for μ_E-almost all $(\boldsymbol{p},\boldsymbol{x})\in\Omega_E$. Thus, after an integration over Ω_E, this together with (4.13) implies that

$$\lim_{\hbar\to 0} S_2(E,\hbar) = 0\ . \tag{4.19}$$

According to a standard argument in the proof of quantum ergodicity for scalar Hamiltonians, see [Zel87, CdV85], the vanishing of $S_2(E,\hbar)$ in the semiclassical limit implies the existence of a density-one subsequence $\{\psi_{k_j}\}_{j\in\mathbb{N}}\subset\{\psi_k\}_{k\in\mathbb{N}}$ such that (4.11) holds. Another standard, diagonal construction then ensures that a subsequence can be chosen that is independent of the observable, see [Zel87, CdV85]. □

5 Discussion

In the case of scalar Hamiltonians quantum ergodicity is often interpreted in terms of Wigner- or Husimitransforms of eigenfunctions. In this context one concludes that along a subsequence of density one the Wigner- or Husimitransforms of eigenfunctions of a quantum ergodic Hamiltonian weakly converge, as distributions or measures, respectively, to

Liouville measure. Thus the lifts of eigenfunctions to phase space become equidistributed on the hypersurface Ω_E of energy E. In the present situation an analogous interpretation first requires to introduce matrix valued Wigner- and Husimitransforms. In general, the Wignertransform of $\psi \in \mathcal{S}'(\mathbb{R}^d) \otimes \mathbb{C}^n$ is given by

$$W[\psi](\boldsymbol{p},\boldsymbol{x}) = \int_{\mathbb{R}^d} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{y}}\, \overline{\psi}\big(\boldsymbol{x} - \frac{1}{2}\boldsymbol{y}\big) \otimes \psi\big(\boldsymbol{x} + \frac{1}{2}\boldsymbol{y}\big)\ \mathrm{d}y\ . \tag{5.1}$$

Then expectation values of observables $\hat{B}$ with symbols $B \in \mathrm{S}^k(1)$ in states described by $\psi \in L^2(\mathbb{R}^d) \otimes \mathbb{C}^n$ read

$$\langle \psi, \hat{B}\psi \rangle = \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathrm{tr}\big(W[\psi](\boldsymbol{p},\boldsymbol{x})\, B(\boldsymbol{p},\boldsymbol{x})\big)\ \mathrm{d}p\, \mathrm{d}x\ . \tag{5.2}$$

In order to convert the statement of Theorem 4.1 into one about the matrix components of Wignertransforms we introduce the special observables $\hat{B}^{(rs)}$ with symbols $B^{(rs)} = b\, E_{rs} \in \mathrm{S}^0(1)$, where b is a real valued function on phase space that is independent of $\hbar$, and the four constant matrices E_{rs} are defined by

$$E_{11} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\ ,\quad E_{12} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\ ,\quad E_{21} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\ ,\quad E_{22} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\ . \tag{5.3}$$

Although the off-diagonal symbols $b\, E_{12}$ and $b\, E_{21}$ are non-hermitian, Theorem 4.1 can be applied to all of the observables $\hat{B}^{(rs)}$ in an obvious manner. Together with the relation (5.2) this then reveals that along the subsequence $\{\psi_{k_j}\}$ of density one specified in the Theorem the matrix components of the Wignertransforms of the eigenfunctions weakly converge, as distributions on $C_0^\infty(\mathbb{R}^d \times \mathbb{R}^d)$, to either Liouville measure or to zero. More specifically,

$$\lim_{j\to\infty} \frac{1}{(2\pi\hbar)^d} W[\psi_{k_j}] = \frac{1}{2} \frac{1}{\mathrm{vol}\,\Omega_E}\, \delta\big(H_{0,s} - E\big)\, \mathbb{1}_2 \tag{5.4}$$

component-wise in $\mathcal{D}'(\mathbb{R}^d \times \mathbb{R}^d)$. In particular, the semiclassical limit of the Wignerdistributions is a scalar multiple of the identity matrix. This means that the 'spin up' and 'spin down' components become identical and equidistributed over the hypersurface of energy E in phase space. Moreover, there occurs no mixture between 'spin up' and 'spin down' components, which can also be seen on the right-hand side of (4.11) since there only the diagonal elements of the principal symbol B_0 contribute.

Upon introducing matrix valued Husimitransforms through

$$H[\psi](\boldsymbol{p},\boldsymbol{x}) = \frac{1}{(\pi\hbar)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} W[\psi](\boldsymbol{q},\boldsymbol{y})\, \mathrm{e}^{-\frac{1}{\hbar}((\boldsymbol{p}-\boldsymbol{q})^2 + (\boldsymbol{x}-\boldsymbol{y})^2)}\ \mathrm{d}q\, \mathrm{d}y\ , \tag{5.5}$$

one can also consider anti-Wick quantisations of symbols $B \in \mathrm{S}^0(1)$. Expectation values of the corresponding anti-Wick operators $\hat{B}_{AW}$ then read in analogy to (5.2)

$$\langle \psi, \hat{B}_{AW}\psi \rangle = \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathrm{tr}\big(H[\psi](\boldsymbol{p},\boldsymbol{x})\, B(\boldsymbol{p},\boldsymbol{x})\big)\ \mathrm{d}p\, \mathrm{d}x\ . \tag{5.6}$$

Since, moreover, for $B \in \mathrm{S}^0(1)$

$$\left\| \hat{B} - \hat{B}_{AW} \right\|_{\mathcal{L}} = O(\hbar) \ , \tag{5.7}$$

one can replace $\hat{B}$ by $\hat{B}_{AW}$ in (4.11) so that Theorem 4.1 implies an analogue of (5.4), i.e.

$$\lim_{j\to\infty} \frac{1}{(2\pi\hbar)^d} H[\psi_{k_j}] \,\mathrm{d}p\,\mathrm{d}x = \frac{1}{2}\,\mathbb{1}_2\,\mathrm{d}\mu_E \ , \tag{5.8}$$

where the convergence has to be understood component-wise as a weak convergence of probability measures on the phase space $\mathbb{R}^d \times \mathbb{R}^d$.

As a further point we now want to discuss whether it is actually necessary to introduce the SU(2)-extension Y^t of the Hamiltonian flow Φ^t, and to require ergodicity of Y^t in order to obtain quantum ergodicity. To this end we provide an example showing that in general it would not suffice to demand only ergodicity of Φ^t. Let us therefore introduce a quantum Hamiltonian $\hat{H}$ of the type introduced in sections 2. – 4. with symbol[1]

$$H(\boldsymbol{p},\boldsymbol{x}) = H_{0,s}(\boldsymbol{p},\boldsymbol{x})\,\mathbb{1}_2 + \hbar\,C(\boldsymbol{p},\boldsymbol{x})\,\sigma_j \ , \tag{5.9}$$

where σ_j is one of the Pauli matrices and $H_{0,s}$ shall be chosen such that Φ^t is ergodic on Ω_E. Now σ_j can obviously also be considered as a bounded self-adjoint operator on $L^2(\mathbb{R}^d)\otimes\mathbb{C}^2$ which commutes with $\hat{H}$; in fact, $\frac{\hbar}{2}\sigma_j$ is the j-th component of the spin observable. Hence, one can introduce joint eigenvectors $\psi_k \in L^2(\mathbb{R}^d)\otimes\mathbb{C}^2$ of $\hat{H}$ and σ_j. Since $\sigma_j^2 = \mathbb{1}_2$, the eigenvalues of σ_j are $\lambda_k = \pm 1$. Introducing $U_j \in \mathrm{U}(2)$ such that $U_j \sigma_j U_j^\dagger$ is diagonal, we can switch to eigenvectors $\varphi_k := U_j \psi_k$ such that

$$\varphi_k = \begin{pmatrix} \varphi_k^{(+)} \\ 0 \end{pmatrix} \quad \text{if} \quad \lambda_k = +1 \qquad \text{and} \qquad \varphi_k = \begin{pmatrix} 0 \\ \varphi_k^{(-)} \end{pmatrix} \quad \text{if} \quad \lambda_k = -1 \ . \tag{5.10}$$

The expectation values of an observable $\hat{B}$ in these eigenvectors φ_k therefore read

$$\langle \varphi_k, \hat{B}\varphi_k \rangle = \begin{cases} (\varphi_k^{(+)}, \hat{B}_{11}\varphi_k^{(+)}) & \text{if } \lambda_k = +1 \ , \\ (\varphi_k^{(-)}, \hat{B}_{22}\varphi_k^{(-)}) & \text{if } \lambda_k = -1 \ , \end{cases} \tag{5.11}$$

where $(\cdot,\cdot)$ denotes the scalar product in $L^2(\mathbb{R}^d)$. Since the subsequences of the φ_k's with $\lambda_k = +1$ and $\lambda_k = -1$, respectively, are each of density one half, quantum ergodicity cannot hold for general observables $\hat{B}$.

On the other hand, the above example does not fulfill the requirements of Theorem 4.1 so that no contradiction occurs. To see this consider the spin transport equation (3.12), which in the present case reads

$$\dot{d}(\boldsymbol{p},\boldsymbol{x},t) + \mathrm{i}\,C(\Phi^t(\boldsymbol{p},\boldsymbol{x}))\,\sigma_j\,d(\boldsymbol{p},\boldsymbol{x},t) = 0 \ , \qquad d(\boldsymbol{p},\boldsymbol{x},0) = \mathbb{1}_2 \ , \tag{5.12}$$

[1] We owe this example to Stefan Keppeler.

and is solved by the expression

$$d(\boldsymbol{p},\boldsymbol{x},t) = \cos(\alpha(\boldsymbol{p},\boldsymbol{x},t))\,\mathbb{1}_2 - \mathrm{i}\,\sin(\alpha(\boldsymbol{p},\boldsymbol{x},t))\,\sigma_j \ , \tag{5.13}$$

where

$$\alpha(\boldsymbol{p},\boldsymbol{x},t) = \int_0^t C(\Phi^s(\boldsymbol{p},\boldsymbol{x}))\ \mathrm{d}s \ . \tag{5.14}$$

The explicit solution (5.13) of the spin transport equation demonstrates that, even if the flow Φ^t on the base manifold Ω_E is ergodic, its SU(2)-extension Y^t cannot be ergodic on the product phase space $\mathcal{M}$. This is due to the fact that with (5.13) one only explores a one dimensional submanifold of the three dimensional group manifold of SU(2). We therefore conclude that in the case of Pauli Hamiltonians ergodicity of Φ^t alone is not a sufficient criterion for quantum ergodicity.

Acknowledgment

We would like to thank Stefan Keppeler and Roman Schubert for useful discussions.

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