Quantum and classical ergodicity of spinning particles

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Abstract

We give a formulation of quantum ergodicity for Pauli Hamiltonians with arbitrary spin in terms of a Wigner-Weyl calculus. The corresponding classical phase space is the direct product of the phase space of the translational degrees of freedom and the two-sphere. On this product space we introduce a combination of the translational motion and classical spin precession. We prove quantum ergodicity under the condition that this product flow is ergodic.

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1 Introduction

Quantum ergodicity describes the equidistribution of eigenfunctions in the semiclassical limit ($\hbar \to 0$), in the sense that almost all expectation values of quantum observables tend to a classical mean value of the corresponding classical observable. In particular, the Wigner functions associated with almost all eigenfunctions of the Hamiltonian become equidistributed on the energy shell in phase space. A sufficient condition for quantum ergodicity to hold is ergodicity of the corresponding classical dynamics, as was first stated by Shnirelman [1]. It is remarkable that quantum ergodicity is one of the few results in quantum chaos for which there exist mathematical proofs; the first complete ones were given by Zelditch [2] and Colin de Verdière [3]. These are results for scalar Hamiltonians, i.e. for the Laplacian on compact manifolds or, more generally, for Schrödinger operators in $\mathbb{R}^d$ [4]. The case of quantum billiards was considered in [5, 6].

If one wants to describe particles with internal degrees of freedom, such as spin, one has to deal with matrix valued Hamiltonians. Since spin is a purely quantum mechanical property, it is a priori not obvious what should serve as the corresponding classical system. In [7] quantum ergodicity for Pauli Hamiltonians with spin $1/2$ was proven under the condition that a combination of the classical translational dynamics and a quantum spin dynamics driven by the translational motion is ergodic. This kind of mixed classical/quantum description in terms of a skew product dynamics arises naturally in the semiclassical analysis of Hamiltonians with spin [8, 9, 10].

Although spin is a genuinely quantum mechanical property, there exists an intuitive classical analogue given by the so-called vector model which provides a picture of spin as a vector of fixed length whose dynamics is similar to that of angular momentum. The mathematical description of this model goes back to Thomas [11], who gave an equation of motion for a classical particle with a magnetic moment precessing in external fields. In a semiclassical analysis of spinning particles various objects can be related to this classical spin precession [12, 9, 13]. In the vector model the equations of motion are of first order in time, and for pure spin precession can be formulated in a Hamiltonian framework. Thus, after suitable normalisation of the spin vector, the unit sphere $S^2$ serves as the phase space of classical spin precession.

Based on ideas of Stratonovich [14], Gracia-Bondía and Várilly [15, 16] developed a Wigner-Weyl calculus for arbitrary spin $j$, in which quantum mechanical observables, i.e. hermitian $(2j + 1) \times (2j + 1)$ matrices, are represented in terms of functions on the phase space $S^2$. We use this description to rephrase the problem of quantum ergodicity for non-relativistic particles with spin and to prove for arbitrary spin the respective statement under the condition that a different skew product of translational and spin dynamics, where now the spin part is given by classical spin precession, is ergodic.

The paper is organised as follows. In section 2 we briefly review properties of the Weyl correspondence for systems with only either translational or spin degrees of freedom. In section 3 we then discuss how in the semiclassical limit of systems with both kinds of degrees of freedom the motion is governed by the skew product dynamics. We also state a corresponding Egorov theorem. Section 4 is devoted to the proof of quantum ergodicity for...
Pauli Hamiltonians with arbitrary spin. Some particular representations of the Wigner-Weyl transform for spinors and a relation between ergodic properties of the two types of skew products are discussed in two appendices.

2 Weyl quantisation and classical limit

The Weyl quantisation of systems in \( \mathbb{R}^d \) without spin, i.e. taking only translational degrees of freedom into account, is based on unitary irreducible representations of the Weyl-Heisenberg operators

\[
\rho(p, q) := e^{\frac{i}{\hbar}(q \hat{P} + p \hat{X})},
\]

where \( \hat{P}_k, \hat{X}_k, k = 1, \ldots, d, \) are momentum and position operators, respectively, satisfying canonical commutation relations. According to the Stone-von Neumann theorem such representations are unitarily equivalent to the Schrödinger representation \( \rho_S(p, q) \) of (2.1) on the Hilbert space \( \mathcal{H}_{\text{trans}} = L^2(\mathbb{R}^d) \), in which \( \hat{X}_k \) is realised as a multiplication operator and \( \hat{P}_k = \frac{\hbar}{i} \frac{\partial}{\partial x_k} \). The Schrödinger representation hence acts on \( \psi \in L^2(\mathbb{R}^d) \) as

\[
(\rho_S(p, q) \psi)(x) = e^{\frac{i}{\hbar}p \cdot (x + \frac{1}{2}q)} \psi(x + q).
\]

See [17] for further details.

A classical observable \( B(p, x) \) is a real valued function on phase space \( \mathbb{R}^d \times \mathbb{R}^d \), to which the Weyl quantisation assigns a symmetric operator \( \hat{B} \) on \( L^2(\mathbb{R}^d) \),

\[
\hat{B} := \frac{1}{(2\pi \hbar)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \tilde{B}(p, q) \rho_S(p, q) \, dp \, dq ,
\]

where

\[
\tilde{B}(p, q) := \frac{1}{(2\pi \hbar)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} B(\xi, z) e^{-\frac{i}{\hbar}(\xi \cdot q + z \cdot p)} \, d\xi \, dz
\]

denotes the Fourier transform of the classical observable. The operation of \( \hat{B} \) on (suitable) \( \psi \in L^2(\mathbb{R}^d) \) then reads

\[
\hat{B} \psi(x) = \frac{1}{(2\pi \hbar)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} e^{\frac{i}{\hbar}p \cdot (x - y)} B(p, \frac{1}{2}(x + y)) \psi(y) \, dy \, dp ,
\]

In fact, \( B \) can even be a (tempered) distribution on phase space, \( B \in S'(\mathbb{R}^d \times \mathbb{R}^d) \); in this case the operator \( \hat{B} \) is defined on the domain \( \mathcal{S}(\mathbb{R}^d) \subset L^2(\mathbb{R}^d) \). Reversing the above reasoning, one notices that the Schwartz kernel theorem allows to represent every continuous linear map \( \hat{B} \) from \( \mathcal{S}(\mathbb{R}^d) \) into \( \mathcal{S}'(\mathbb{R}^d) \) as a Weyl operator (2.3) with symbol \( B(p, x) \), which in general is a distribution on phase space (see, e.g., [17]). The map \( \hat{B} \mapsto B(p, x) \) can be
made more explicit if \( \hat{B} \) is a trace class operator on \( L^2(\mathbb{R}^d) \). Since \( \rho_S(p, q) \) is bounded, \( \hat{B} \rho_S(p, q) \) is also of trace class, and

\[
\hat{B}(p, q) = \text{Tr}(\hat{B} \rho_S(p, q)) ,
\]

(2.6)

where \( \text{Tr}(\cdot) \) denotes the operator trace on \( \mathcal{H}_{\text{trans}} \). We remark that the symbol of a Weyl operator can in principle depend on \( \hbar \). In such a case a direct interpretation of \( B(p, x) \) as a classical observable is inappropriate. However, if one restricts the class of observables suitably, the symbols possess asymptotic expansions as \( \hbar \to 0 \),

\[
B(p, x; \hbar) \sim \sum_{k \geq 0} \hbar^k B_k(p, x) ;
\]

(2.7)

for the precise meaning of (2.7) see, e.g., [18, 19]. Now the principal symbol \( B_0(p, x) \) is a function on phase space independent of \( \hbar \) that serves as the corresponding classical observable.

Summarising its most important properties, the Weyl quantisation can be characterised by the following properties (see, e.g., [17, 18, 19]):

(i) The map \( \hat{B} \mapsto B(p, x) \) is linear.

(ii) \( \hat{B}^\dagger \mapsto \overline{B(p, x)} \).

(iii) If \( \hat{B} \) is of trace class, then

\[
\text{Tr} \hat{B} = \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} B(p, x) \, dp \, dx .
\]

(2.8)

(iv) Covariance: If \( G \in \text{Sp}(2d, \mathbb{R}) \) is a linear canonical transformation with metaplectic representation \( \pi_M(G) \), then \( \hat{B} \mapsto B(p, x) \) implies

\[
\pi_M(G)^\dagger \hat{B} \pi_M(G) \mapsto B(G(p, x)) .
\]

(2.9)

We now turn attention to a quantum mechanical spin, without translational degrees of freedom. Its (pure) states are described by vectors in the Hilbert space \( \mathcal{H}_{\text{spin}} = \mathbb{C}^{2j+1} \), where \( j \in \frac{1}{2} \mathbb{N} \) denotes the (fixed) spin quantum number. Spin observables are therefore hermitian \( (2j + 1) \times (2j + 1) \) matrices. The corresponding classical phase space is given by the two-sphere \( S^2 \), considered as a symplectic manifold whose symplectic structure is provided by the area two-form. In spherical coordinates \((\theta, \varphi)\) for \( S^2 \) a symplectic chart is given by \((p, q) = (\cos \theta, \varphi) \in (-1, 1) \times (0, 2\pi) \). For reasons of convenient normalisation we here choose the symplectic two-form as

\[
\omega(p, q) := \frac{1}{\hbar \sqrt{j(j+1)}} \, dp \wedge dq = \frac{1}{\hbar \sqrt{j(j+1)}} \sin \theta \, d\theta \wedge d\varphi .
\]

(2.10)
In the following we will often denote points of $S^2$ by $n \in \mathbb{R}^3$ with $|n| = 1$ so that in spherical coordinates $n = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)^T$. In these coordinates the normalised area two-form is given by $d\mu_{S^2}(n) = \frac{1}{4\pi} \sin \theta \, d\theta \wedge d\varphi$. Below we will show that the quantum mechanical spin operator $\hat{S}$ is then associated with the vector $s := \hbar \sqrt{j(j+1)} n \in \mathbb{R}^3$ of length $\hbar \sqrt{j(j+1)}$; in other words, $n = s/|s| \in S^2$ represents a normalised ‘classical’ spin vector.

A Weyl correspondence for spin, with properties as close as possible to the ones discussed above in the case of translational degrees of freedom, has to assign a real valued function on $S^2$ to a hermitian $(2j+1) \times (2j+1)$ matrix in such a way that properties analogous to (i)–(iv) of above hold. Based on ideas of Stratonovich [14], Várilly and Gracia-Bondía [15, 16] have constructed such a Weyl correspondence. In their approach quantum mechanical observables $\hat{b}$ are represented as

$$
\hat{b} = (2j+1) \int_{S^2} b(n) \hat{\Delta}_j(n) \, d\mu_{S^2}(n) .
$$

(2.11)

Here $\hat{\Delta}_j(n)$ is a function on $S^2$ taking values in the hermitian $(2j+1) \times (2j+1)$ matrices, and the symbol $b(n) \in L^2(S^2)$ can be obtained from the observable $\hat{b}$ in analogy to (2.6),

$$
b(n) = \text{tr} \left( \hat{b} \hat{\Delta}_j(n) \right) ,
$$

(2.12)

with $\text{tr}(\cdot)$ meaning the matrix trace. In [16] it is shown that there are $2^{2j}$ possibilities for a Weyl correspondence with a kernel $\hat{\Delta}_j(n)$ that fulfills

(a) $\hat{\Delta}_j(n)^\dagger = \hat{\Delta}_j(n)$ for all $n \in S^2$.

(b) $(2j+1) \int_{S^2} \hat{\Delta}_j(n) \, d\mu_{S^2}(n) = 1_{2j+1}$.

(c) Covariance: If $g \in SU(2)$ and $\pi_j$ denotes the $(2j+1)$-dimensional unitary irreducible representation of $SU(2)$, then $\hat{\Delta}_j(\varphi(g)n) = \pi_j(g) \hat{\Delta}_j(n) \pi_j(g)^\dagger$.

In the covariance property of the kernel $\varphi$ denotes the covering map from $SU(2)$ to $SO(3)$: For every $g \in SU(2)$ one defines the adjoint map $\text{Ad}_g$ as the linear map of the Lie algebra $su(2)$ given by $X \mapsto g^\dagger X g$. Expanding $X \in su(2)$ in terms of the Pauli matrices, $X = x \cdot \sigma$, $x \in \mathbb{R}^3$, the adjoint map operates as $\text{Ad}_g(x \cdot \sigma) = (\varphi(g)x) \cdot \sigma$. In this way every $g \in SU(2)$ is mapped to some $\varphi(g) \in SO(3)$; in fact this map is two-to-one and provides the universal covering of $SO(3)$ by $SU(2)$. Hence $\varphi(g)n$ means the rotation of $n \in \mathbb{R}^3$ (with $|n| = 1$) by $\varphi(g) \in SO(3)$. In [16] one choice out of the $2^{2j}$ possibilities to define $\hat{\Delta}_j(n)$ is singled out due to its connection with spin-coherent states; however, for our purposes this particular choice is not important and, thus, will not be specified here. For illustration, some explicit examples are shown in appendix A.

The properties (a)–(c) of $\hat{\Delta}_j(n)$ listed above now imply properties of the symbols $b(n)$ that are closely analogous to those of symbols in the case of translational degrees of freedom:
(i) The map \( \hat{b} \mapsto b(n) \) is linear.

(ii) \( \hat{b}^\dagger \mapsto b(n) \).

(iii) \( \text{tr} \hat{b} = (2j + 1) \int_{S^2} b(n) \, d\mu_{S^2}(n) \).

(iv) For every \( g \in \text{SU}(2) \): \( \pi_j(g)^\dagger \hat{b} \pi_j(g) \mapsto b(\varphi(g)n) \).

In addition one obtains the simple relation

\[
\text{tr}(\hat{a} \hat{b}) = (2j + 1) \int_{S^2} a(n) b(n) \, d\mu_{S^2}(n)
\]

for the trace of a matrix product.

The covariance of the quantisation as expressed by (iv) relates the quantum mechanical
time evolution of a spin to a classical dynamics (see also [10]): Let \( d\pi_j \) denote the \((2j + 1)\)-
dimensional derived representation of \( \text{su}(2) \), i.e. \( d\pi_j(X) = \frac{1}{i} \frac{d}{d\lambda} \pi_j(e^{i\lambda X})|_{\lambda = 0} \). Then the
spin operators \( \hat{S}_k \), \( k = 1, 2, 3 \), are given by \( \hat{S}_k = \frac{i}{2} d\pi_j(\sigma_k) \), with commutation relations
\( [\hat{S}_k, \hat{S}_l] = i\hbar \varepsilon_{klm} \hat{S}_m \). The Weyl correspondence now assigns the vector valued symbol \( s = \hbar \sqrt{j(j + 1)} n \) to the vector \( \hat{S} \) of these quantum mechanical spin operators, see appendix A.

A typical (time independent) quantum Hamiltonian is given by

\[
\hat{H}_{\text{spin}} = \hat{S} \cdot C = \frac{\hbar}{2} C \cdot d\pi_j(\sigma) ,
\]

where \( C \in \mathbb{R}^3 \) is some constant vector. This Hamiltonian generates a quantum mechanical
time evolution that is governed by the unitary operators

\[
e^{-\frac{i}{\hbar} \hat{H}_{\text{spin}} t} = \pi_j(e^{-\frac{i}{\hbar} C \cdot \sigma t}) ,
\]

so that a time evolved observable reads

\[
\hat{b}(t) = e^{\frac{i}{\hbar} \hat{H}_{\text{spin}} t} \hat{b} e^{-\frac{i}{\hbar} \hat{H}_{\text{spin}} t} = \pi_j(e^{-\frac{i}{\hbar} C \cdot \sigma t})^\dagger \hat{b} \pi_j(e^{-\frac{i}{\hbar} C \cdot \sigma t}) .
\]

If \( b(n) \) is the classical observable associated with \( \hat{b} \), the relation \( (2.16) \) and the covariance
property (iv) hence assign the classical observable

\[
b(t)(n) = b(\varphi(e^{-\frac{i}{\hbar} C \cdot \sigma t})n)
\]

to \( \hat{b}(t) \). In this way one is provided with a dynamics \( n \mapsto n(t) = \varphi(e^{-\frac{i}{\hbar} C \cdot \sigma t})n \) on \( S^2 \) that
is governed by the equations of motion

\[
\dot{n}(t) = C \times n(t)
\]

describing a precession of \( n(t) \) about \( C \). On the other hand, the Weyl correspondence
associates the classical Hamiltonian \( H_{\text{spin}}(n) = s \cdot C \) to the quantum Hamiltonian \( (2.14) \).
Together with the Poisson bracket \( \{ \cdot, \cdot \}_{S^2} \) derived from the symplectic structure on \( S^2 \) given by \( \omega \) one therefore identifies (2.18) as the equations of motion generated by \( H_{\text{spin}} \), i.e.

\[
\dot{n}(t) = \{ H_{\text{spin}}, n(t) \}_{S^2} = C \times n(t).
\]  

(2.19)

Thus the assignment (2.12) of a function on \( S^2 \) to a quantum observable commutes with the (quantum mechanical or classical, respectively) time evolution, see also appendix B. This property is a special feature of the Weyl correspondence for spin. In the case of translational degrees of freedom the analogous relation, known as the Egorov theorem [20], only holds for the assignment of the principal symbol \( B_0(p, x) \), and not of the full symbol \( B(p, x) \), to a quantum observable.

### 3 Coupling of spin and translational motion

The quantum mechanical description of particles with spin requires to couple translational and spin degrees of freedom. The relevant Hilbert space \( \mathcal{H} \) therefore has to be the tensor product of \( \mathcal{H}_{\text{trans}} \) and \( \mathcal{H}_{\text{spin}} \), i.e. \( \mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathbb{C}^{2j+1} \). The state vectors of a spinning particle are hence \( (2j+1) \)-component spinors whose components are square integrable over \( \mathbb{R}^d \).

Observables are represented by self-adjoint operators on \( \mathcal{H} \), which in Weyl representation read

\[
\hat{B}\psi(x) = \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} e^{\frac{i}{\hbar} p \cdot (x-y)} B(p, \frac{1}{2}(x+y)) \psi(y) \, dy \, dp.
\]

(3.1)

Here the symbol \( B(p, x) \) is in general a \( (2j+1) \times (2j+1) \) matrix valued distribution on phase space \( \mathbb{R}^d \times \mathbb{R}^d \). The operators (3.1) then act on \( \psi \in S(\mathbb{R}^d) \otimes \mathbb{C}^{2j+1} \).

In a non-relativistic context the quantum dynamics is generated by the (Pauli) Hamiltonian

\[
\hat{H}_P = \hat{H}_{\text{trans}} \mathbb{1}_{2j+1} + \frac{\hbar}{2} \mathbb{d}\pi_j(\sigma) \cdot \hat{C}
\]

(3.2)

that consists of a scalar part \( \hat{H}_{\text{trans}} \) describing the dynamics of the translational degrees of freedom, and a genuinely matrix valued part that contains a coupling of spin to the translational motion; here \( \hat{C}_k \) are Weyl quantisations of suitable functions \( C_k(p, x) \) on phase space. Typically, \( \hat{H}_{\text{trans}} \) is of the form

\[
\hat{H}_{\text{trans}} = \frac{1}{2m} \left( \frac{\hbar}{i} \nabla - e \frac{c}{c} A(x) \right)^2 + e\phi(x),
\]

(3.3)

with (static) electromagnetic potentials \( A, \phi \), i.e. it is a Weyl quantisation of the classical Hamiltonian

\[
H_0(p, x) = \frac{1}{2m} \left( p - e \frac{c}{c} A(x) \right)^2 + e\phi(x).
\]

(3.4)
Examples for the coupling of spin to the translational motion are given by a coupling to an external magnetic field,
\[ C(p, x) = -\frac{e}{2mc} B(x), \]
or a spin-orbit coupling
\[ C(p, x) = \frac{1}{4m^2c^2|x|} \frac{d\Phi|}{d|x|} (x \times p). \]
For the following the specific form of the Hamiltonian, however, is not relevant. We only require \( H_0(p, x) \) to fulfill certain criteria that guarantee \( \hat{H}_P \) to be (essentially) self-adjoint, bounded from below, and to possess a purely discrete spectrum in some interval \([E - \varepsilon, E + \varepsilon]\). For details see [7].

For simplicity the further observables that we are going to consider shall be bounded Weyl operators on \( \mathcal{H} \). Their symbols are smooth, matrix valued functions on phase space, which may also depend on \( \hbar \) in such a way that an asymptotic expansion \( (\hbar \to 0) \)
\[ B(p, x; \hbar) \sim \sum_{k \geq 0} \hbar^k B_k(p, x) \] 
(3.5)
analogous to (2.7) holds (see [7] for further details). As far as the translational degrees of freedom are concerned, the classical observable corresponding to \( \hat{B} \) is then given by its principal symbol
\[ B_0(p, x), \]
whose symbol
\[ J(p, x) = (x \times p) \mathbb{1}_{2j+1} + \hbar \frac{1}{2} d\pi_j(\sigma) \] 
(3.6)
has a principal part that consists of orbital angular momentum, and a sub-principal part given by spin.

The relation between the quantum and classical time evolution, i.e. the relevant Egorov theorem, has in this context been derived in [8]. In order to state this version of the Egorov theorem, let \( d(p, x, t) \in SU(2) \) be the solution of the spin-transport equation \[ \dot{d}(p, x, t) + \frac{i}{2} C(\Phi^t(p, x)) \cdot \sigma \ d(p, x, t) = 0 \] with \( d(p, x, 0) = \mathbb{1}_2 \),
(3.7)
where \( \Phi^t(p, x) = (p(t), x(t)) \) denotes the classical flow on the phase space \( \mathbb{R}^d \times \mathbb{R}^d \) generated by the classical translational Hamiltonian \( H_0(p, x) \), i.e. \( (p(t), x(t)) \) are solutions of Hamilton’s equations of motion with initial condition \( (p(0), x(0)) = (p, x) \). Hence, a comparison with (2.15) reveals that \( \pi_j(d(p, x, t)) \) is the quantum mechanical propagator for the spin degrees of freedom along the trajectories \( \Phi^t(p, x) \) of the classical translational motion. The Egorov theorem relevant in the present situation now states that the time evolution \( \hat{B}(t) \), generated by a Pauli Hamiltonian (3.2), of an observable (3.1) with a symbol allowing for an asymptotic expansion (3.5), is again an operator of the same type and its principal symbol \( B_0(t)(p, x) \) reads
\[ B_0(t)(p, x) = \pi_j(d(p, x, t)) \hat{B}_0(\Phi^t(p, x)) \pi_j(d(p, x, t)). \] 
(3.8)
In this expression the translational degrees of freedom are obviously propagated classically by means of the flow \( \Phi^t \). In contrast, a glance at the relation (2.16) reveals that the
dynamics of the spin degrees of freedom are genuinely quantum mechanical, but are driven by the classical translational flow and take place along the trajectories of this flow. This observation reflects the mixed (classical/quantum) level of description of the translational and spin degrees of freedom.

We now proceed to describe spin within the framework of the Weyl correspondence outlined in the previous section. Thus, according to (3.1) and (2.11) quantum mechanical observables \( \hat{B} \) are represented as

\[
\hat{B}\psi(x) = \frac{2j+1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} \int_{S^2} e^{i p \cdot (x-y)} b(p, \frac{1}{2}(x+y), n) \hat{\Delta}_j(n) \psi(y) \, dy \, dp \, d\mu_S(n),
\]

where according to (2.12)

\[
b(p, x, n) = \text{tr}(B(p, x) \hat{\Delta}_j(n))
\]

is the associated scalar symbol; e.g., in the case of the operator \( \hat{J} \) of total angular momentum the scalar symbol related to the matrix valued one (3.4) is given by

\[
j(p, x, n) = x \times p + \hbar j (j+1) n.
\]

When applied to the principal symbol \( B_0(p, x) \), the relation (3.10) now associates with every quantum observable \( \hat{B} \) of the type under consideration a classical observable \( b_0(p, x, n) \), which is a function on the combined phase space \( \mathbb{R}^d \times \mathbb{R}^d \times S^2 \). In particular, the Egorov theorem can be brought into the following form: According to (3.8) the matrix valued principal symbol of \( \hat{B}(t) \) is of the same type as the right-hand side of (2.10). Hence, due to the covariance property of the spin-Weyl correspondence with respect to \( SU(2) \), the associated scalar principal symbol \( b_0(t)(p, x, n) = \text{tr}(B_0(t)(p, x) \hat{\Delta}_j(n)) \) reads

\[
b_0(t)(p, x, n) = b_0(\Phi^t(p, x), \varphi(d(p, x, t))n) = b_0(p(t), x(t), n(t)).
\]

The classical observable corresponding to the quantum observable \( \hat{B}(t) \) at time \( t \) therefore follows from the respective classical observable at time zero by a purely classical time evolution on the combined phase space of translational and spin degrees of freedom. The combined flow on \( \mathbb{R}^d \times \mathbb{R}^d \times S^2 \), denoted as \( Y^t_{cl} \), is therefore given by the skew product,

\[
Y^t_{cl}(p, x, n) := (\Phi^t(p, x), \varphi(d(p, x, t))n) = (p(t), x(t), n(t)),
\]

and the scalar Egorov relation (3.12) reads

\[
b_0(t)(p, x, n) = b_0(Y^t_{cl}(p, x, n)).
\]

See, e.g., [21] for a general discussion of skew products. The spin part \( n \mapsto n(t) = \varphi(d(p, x, t))n \) of the combined classical dynamics takes place along the trajectories \( \Phi^t(p, x) \) of the translational motion and describes a precession of \( n(t) \) about the instantaneous axis \( C(\Phi^t(p, x)) \), compare (2.18). This is a non-relativistic version of the Thomas precession of spin [11].
4 Quantum ergodicity

Quantum ergodicity for Pauli Hamiltonians of the form (3.2) with spin 1/2 was derived in [7] under the condition that the underlying mixed classical/quantum system be ergodic. For this purpose, the two dynamics inherent in (3.8) had to be combined into a single skew product flow $Y^t$ on $\mathbb{R}^d \times \mathbb{R}^d \times SU(2)$ via

$$Y^t((p,x),g) := (\Phi^t(p,x), d(p,x,t)g), \quad (p,x) \in \mathbb{R}^d \times \mathbb{R}^d \times SU(2),$$

(4.1)

see also [10] for further details. Introducing Liouville measure (the microcanonical distribution)

$$d\mu_E(p,x) := \frac{1}{\text{vol } \Omega_E} \delta(H_0(p,x) - E) \, dp \, dx$$

(4.2)

on the energy shell

$$\Omega_E := \{(p,x) \in \mathbb{R}^d \times \mathbb{R}^d \mid H_0(p,x) = E\},$$

(4.3)

one observes that $Y^t$ leaves the product measure $\mu := \mu_E \times \mu_H$ invariant, where $\mu_H$ denotes the normalised Haar measure on SU(2). Now ergodicity of $Y^t$ on $\Omega_E \times SU(2)$ with respect to $\mu$ means that for every integrable function $F \in L^1(\Omega_E \times SU(2), d\mu)$ the relation

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T F(Y^t(\xi,y,h)) \, dt = \int_{\Omega_E \times SU(2)} F(p,x,g) \, d\mu(p,x,g)$$

(4.4)

holds for $\mu$-almost all initial conditions $(\xi,y,h) \in \Omega_E \times SU(2)$. Provided that ergodicity of $Y^t$ and certain properties of the principal symbol $H_0$ of the quantum Hamiltonian hold, it was shown in [7] that in every sequence $\{\psi_k \mid E_k \in I(E,\hbar)\}$ of orthonormal eigenspinors of the Hamiltonian $H_P$ with eigenvalues $E_k$ in an interval $I(E,\hbar) := [E - \hbar \omega, E + \hbar \omega]$, which shall not contain any critical values of $H_0$, there exists a sub-sequence $\{\psi_{k_\nu} \mid E_{k_\nu} \in I(E,\hbar)\}$ of density one, i.e.

$$\lim_{\hbar \to 0} \frac{\#\{\nu \mid E_{k_\nu} \in I(E,\hbar)\}}{\#\{k \mid E_k \in I(E,\hbar)\}} = 1,$$

(4.5)

such that for every quantum observable $\hat{B}$ with hermitian symbol $B(p,x)$ and principal symbol $B_0(p,x)$ the expectation values taken in the eigenstates $\{\psi_{k_\nu}\}_{\nu \in \mathbb{N}}$ of $H_P$ fulfill

$$\lim_{\nu \to \infty} \langle \psi_{k_\nu}, \hat{B} \psi_{k_\nu} \rangle = \frac{1}{2} \text{tr} \int_{\Omega_E} B_0(p,x) \, d\mu_E(p,x) =: \frac{1}{2} \text{tr} \mu_E(B_0).$$

(4.6)

Moreover, the sub-sequence $\{\psi_{k_\nu}\}_{\nu \in \mathbb{N}}$ can be chosen independent of the observable $\hat{B}$. Here we remark that since the number $N_I$ of eigenvalues $E_k \in I(E,\hbar)$ grows like

$$N_I \sim 2\hbar \omega \frac{(2j + 1) \text{vol } \Omega_E}{(2\pi \hbar)^d},$$

(4.7)
(see [10, 7]) in the semiclassical limit, both the numerator and the denominator in (4.3) become infinite as $\hbar \to 0$. Thus, the limit $\nu \to \infty$ in (4.6) requires the semiclassical limit.

We will now derive the analogous result for Pauli Hamiltonians with arbitrary spin under the condition that $Y^l_{\text{cl}}$, i.e. the purely classical skew product (3.13), is ergodic on $\Omega_E \times S^2$ with respect to the invariant measure $\mu_{\text{cl}} := \mu_E \times \mu_{S^2}$. This means that for every integrable function $f \in L^1(\Omega_E \times S^2, d\mu_{\text{cl}})$ the relation

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T f(Y^l_{\text{cl}}(\xi, y, m)) \, dt = \int_{\Omega_E \times SU(2)} f(p, x, n) \, d\mu_{\text{cl}}(p, x, n)$$

holds for $\mu_{\text{cl}}$-almost all initial conditions $(\xi, y, m) \in \Omega_E \times S^2$. We remark that the ergodicity (4.3) of $Y^l_{\text{cl}}$, which was required for quantum ergodicity in [7], implies the relation (4.8), i.e. ergodicity of $Y^l_{\text{cl}}$, see appendix B. Also notice that using property (iii) on page 5, the right-hand side of (4.6) can be rewritten as

$$\frac{1}{2} \text{tr} \mu_E(B_0) = \int_{\Omega_E \times S^2} b_0(p, x, n) \, d\mu_{\text{cl}}(p, x, n) =: \mu_{\text{cl}}(b_0).$$

In order to prove quantum ergodicity for arbitrary spin $j$ along the lines of [22, 3, 7], we now analyse the quantity

$$S_2(E, \hbar) := \frac{1}{N_I} \sum_{E_k \in I(E, \hbar)} \left| \langle \psi_k, \hat{B}\psi_k \rangle - \mu_{\text{cl}}(b_0) \right|^2,$$

which is the variance of the expectation values of the quantum observable $\hat{B}$ about the classical mean of its scalar principal symbol $b_0$. Introducing the bounded and self-adjoint auxiliary operator

$$\hat{B}_T := \frac{1}{T} \int_0^T e^{i-H_{P^T} t} \hat{B} e^{-i-H_{P^T} t} \, dt - \mu_{\text{cl}}(b_0) \mathbb{1}_{2j+1},$$

the variance (4.10) also reads

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

where the estimate on the right-hand side follows from the Cauchy-Schwarz inequality. Quantum ergodicity is now implied, if this upper bound vanishes in the semiclassical limit. In order to show that this indeed happens, we employ the Szegö limit formula

$$\lim_{\hbar \to 0} \frac{1}{N_I} \sum_{E_k \in I(E, \hbar)} \langle \psi_k, \hat{B}\psi_k \rangle = \frac{1}{2j + 1} \text{tr} \mu_E(B_0) = \mu_{\text{cl}}(b_0)$$

for an observable $\hat{B}$, which has been established in [7]. This formula is valid under certain technical assumptions on the symbol of the Hamiltonian $H_P$ (see [3] for details), and
if the periodic orbits of the translational flow $\Phi^t$ with non-trivial periods form a set of Liouville measure zero in $\Omega_E$. Since $Y^t_{cl}$ shall be ergodic, which includes the ergodicity of the translational motion on the energy shell $\Omega_E$, this condition is clearly fulfilled and we can apply (4.13) to (4.12), yielding

$$\lim_{\hbar \to 0} S_2(E, \hbar) \leq \frac{1}{2j + 1} \text{tr} \mu_E((B_{T,0})^2) = \mu_{cl}((b_{T,0})^2),$$

(4.14)

where on the right-hand side use has been made of the relation (2.13). Here $B_{T,0}(p, x)$ and $b_{T,0}(p, x, n)$ denote the matrix valued and scalar principal symbol, respectively, of the auxiliary operator (4.11).

In order to conclude the proof consider the scalar principal symbol $b_{T,0}$ of $\hat{B}_T$, which according to (4.11) and (3.14) reads

$$b_{T,0}(p, x, n) = \frac{1}{T} \int_0^T b_0(Y^t_{cl}(p, x, n)) \, dt - \mu_{cl}(b_0).$$

(4.15)

An application of the ergodicity (4.8) of $Y^t_{cl}$ to the principal symbol $b_0(p, x, n)$ of the observable $\hat{B}$ now reveals that $b_{T,0}(p, x, n)$ vanishes as $T \to \infty$ for $\mu_{cl}$-almost all $(p, x, n) \in \Omega_E \times S^2$. Since therefore the right-hand side of (4.14) vanishes, this finally implies that

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

(4.16)

According to a general construction in proofs of quantum ergodicity [3, 2], the vanishing of $S_2(E, \hbar)$ in the semiclassical limit implies the existence of a density-one sub-sequence $\{\psi_{k_\nu}\}_{\nu \in \mathbb{N}} \subset \{\psi_k\}_{k \in \mathbb{N}}$ along which one has

$$\lim_{\nu \to \infty} \langle \psi_{k_\nu}, \hat{B}\psi_{k_\nu} \rangle = \mu_{cl}(b_0).$$

(4.17)

Finally, a diagonal construction (see again [3, 2]) yields a sub-sequence, still of density one, that is independent of the observable $\hat{B}$ such that (4.17) holds along this sub-sequence for all observables of the type considered here.

Our conclusion therefore is that quantum ergodicity for Pauli Hamiltonians with arbitrary spin $j$ holds under the condition that the classical skew product $Y^t_{cl}$ of translational and spin dynamics is ergodic on $\Omega_E \times S^2$. We remark that ergodicity of $Y^t_{cl}$ implies ergodicity of the translational motion $\Phi^t$ on the energy shell $\Omega_E$. However, ergodicity of $\Phi^t$ alone is not a sufficient condition for quantum ergodicity; see [4] for a counter-example.

For the purpose of an interpretation of the quantum ergodicity relation (4.17) for Pauli Hamiltonians with arbitrary spin, we now discuss its effect in terms of Wigner transforms of spinors $\psi \in S'(\mathbb{R}^d) \otimes \mathbb{C}^{2j+1}$. Matrix valued Wigner transforms are defined as

$$W[\psi](p, x) := \int_{\mathbb{R}^d} e^{-\frac{i}{\hbar}py} \psi(x - \frac{1}{2}y) \otimes \psi(x + \frac{1}{2}y) \, dy,$$

(4.18)
so that quantum expectation values of an observable $\hat{B}$ with symbol $B(p, x)$ in states given by $\psi \in L^2(\mathbb{R}^d) \otimes \mathbb{C}^{2j+1}$ read

$$\langle \psi, \hat{B} \psi \rangle = \frac{1}{(2\pi \hbar)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \text{tr} (W[\psi](p, x) B(p, x)) \, dp \, dx .$$

(4.19)

After employing the relation (2.13) we obtain

$$\langle \psi, \hat{B} \psi \rangle = \frac{2j + 1}{(2\pi \hbar)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \int_{S^2} w[\psi](p, x, n) b(p, x, n) \, dp \, dx \, d\mu_{S^2}(n) ,$$

(4.20)

where

$$w[\psi](p, x, n) := \text{tr} \left( W[\psi](p, x) \hat{\Delta}_j(n) \right)$$

(4.21)

is introduced as a scalar Wigner transform of $\psi \in S'(\mathbb{R}^d) \otimes \mathbb{C}^{2j+1}$. In this context, quantum ergodicity (4.17) implies that along a density-one sub-sequence the scalar Wigner transforms $\{w[\psi_{k_\nu}]\}_{\nu \in \mathbb{N}}$ of eigenspinors of the quantum Hamiltonian become equidistributed on both the (translational) energy shell $\Omega_E$ and on the classical phase space $S^2$ of spin, i.e.

$$\lim_{\nu \to \infty} \frac{2j + 1}{(2\pi \hbar)^d} w[\psi_{k_\nu}](p, x, n) = \frac{1}{\text{vol} \Omega_E} \delta(H_0(p, x) - E) ,$$

(4.22)

where the convergence has to be understood in the sense of distributions, i.e. after integration with a suitable function on $\mathbb{R}^d \times \mathbb{R}^d \times S^2$ as in (4.20).

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**A  Explicit form of the kernel $\hat{\Delta}_j(n)$**

In this appendix we comment on some properties of the particular representation for the kernel $\hat{\Delta}_j(n)$ that was chosen in [16] and give explicit examples for $j = \frac{1}{2}$ and $j = 1$.

Expressing $n \in S^2 \subset \mathbb{R}^3$ in spherical coordinates, $n = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)^T$, we denote the usual spherical harmonics by $Y_{lm}(n)$. Then the kernel $\hat{\Delta}_j(n)$ can be expanded in the basis $\{Y_{lm}(n) \mid l \in \mathbb{N}_0, |m| \leq l\}$,

$$\hat{\Delta}_j(n) = \sum_{l=0}^{2j} \sum_{m=-l}^{l} \sqrt{\frac{4\pi}{2j + 1}} C_{lm}^j Y_{lm}(n) ,$$

(A.1)

where for given $j$ the $C_{lm}^j$ are $(2j + 1) \times (2j + 1)$ matrices, see [16] for details. Notice that this expansion terminates at $l = 2j$. 

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Thus, if one expands a general classical observable, given by some function \( b(n) \in L^2(S^2) \), in spherical harmonics and uses the spin-Weyl correspondence (2.11) in order to associate to it a spin-\( j \) quantum observable \( \hat{b} \), then its Weyl symbol (2.12) will in general not coincide with the original \( b(n) \), but instead its expansion in spherical harmonics will be truncated at \( l = 2j \). However, since the fundamental theory is quantum mechanics, one should adopt the reverse point of view: Starting from a spin-\( j \) quantum observable \( \hat{b} \) one can assign to it its Weyl symbol \( b(n) \), given by (2.12), as a classical observable. Then by (2.11) this correspondence is one-to-one.

Therefore, in a classical description of a spin \( j \) a general observable \( b(n) \in L^2(S^2) \) has an expansion in spherical harmonics \( Y_{lm}(n) \) which terminates at \( l = 2j \). Conversely, if the aim were a complete quantum description of a top whose classical dynamics is given by the Euler equations (instead of a classical description of, say, an electron with fixed spin \( \frac{1}{2} \)), one would have to perform the semiclassical limit \( \hbar \to 0 \) simultaneously with the limit of large spin, \( j \to \infty \), such that \( j\hbar = O(1) \), cf., e.g., [23].

As an explicit example we now briefly discuss some properties of \( \hat{\Delta}_j(n) \) in the representation chosen in [10]. For spin \( j = \frac{1}{2} \) we obtain

\[
\hat{\Delta}_{1/2}(n) = \sqrt{\pi} \begin{pmatrix} Y_{00}(n) + Y_{10}(n) & -\sqrt{2} Y_{11}(n) \\ -\sqrt{2} Y_{11}(n) & Y_{00}(n) - Y_{10}(n) \end{pmatrix} = \frac{1}{2} \mathbb{1}_2 + \sqrt{\frac{3}{4}} n \cdot \sigma. \tag{A.2}
\]

Since every observable \( \hat{b} \) of a spin \( 1/2 \) is a hermitian \( 2 \times 2 \) matrix, which can be represented as \( \hat{b} = b_0 \mathbb{1}_2 + b \cdot \sigma \) with \( b_0 \in \mathbb{R} \) and \( b \in \mathbb{R}^3 \), the associated classical observable reads

\[
b(n) = \text{tr}(\hat{b} \hat{\Delta}_{1/2}(n)) = b_0 + \sqrt{3} b \cdot n = b_0 + 2\sqrt{j(j+1)} b \cdot n. \tag{A.3}
\]

In particular, the spin operator \( \hat{S} = \frac{\hbar}{2} \sigma \) is mapped to the symbol \( s = \hbar \sqrt{3/4} n \). This last statement generalises to arbitrary spin, i.e. \( \hat{S} = \frac{\hbar}{2} \text{d}\pi_j(\sigma) \) is always mapped to \( s = \hbar \sqrt{j(j+1)} n \). E.g., for \( j = 1 \) the inverse transformation (2.11) reads

\[
\hat{S} = 3 \int_{S^2} s \hat{\Delta}_1(n) \, d\mu_{S^2}(n)
= \frac{\hbar}{2} \begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i\sqrt{2} & 0 \\ i\sqrt{2} & 0 & -i\sqrt{2} \\ 0 & i\sqrt{2} & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{pmatrix}^T, \tag{A.4}
\]

where now the kernel \( \hat{\Delta}_1(n) \) can be expressed as

\[
\hat{\Delta}_1(n) = \frac{1-\sqrt{10}}{3} \mathbb{1}_3 + \frac{\sqrt{2}}{4} (\text{d}\pi_1(\sigma) \cdot n) + \frac{\sqrt{10}}{8} (\text{d}\pi_1(\sigma) \cdot n)^2. \tag{A.5}
\]

**B  Ergodicity of \( Y^t \) and \( Y^t_{\text{cl}} \)**

In this appendix we discuss the relation between the two skew products \( Y^t \) (4.1) and \( Y^t_{\text{cl}} \) (3.13) and their respective ergodic properties.
To this end we need a mapping of quantum spin precession on SU(2) to classical spin precession on $S^2$. This is conveniently given by the Hopf map, one of whose possible realisations reads

$$
\pi_H : \text{SU}(2) \rightarrow S^2 \\
g \mapsto u^T g^1 \sigma^u,
$$

where $u \in \mathbb{C}^2$ with $\|u\|_{\mathbb{C}^2} = 1$ is arbitrary but fixed. We now want to relate the spin part $g \mapsto d(p, x, t)g$ of the skew product flow $Y^t$ to the spin part $n \mapsto \varphi(d(p, x, t))n$ of $Y^t_{\text{cl}}$. The definition of the universal covering map $\varphi : \text{SU}(2) \rightarrow \text{SO}(3)$ implies that

$$
\pi_H(d(p, x, t)g) = \varphi(d(p, x, t)) \pi_H(g),
$$

so that the projection of the (quantum mechanical) time evolution in SU(2) to $S^2$ fulfills the classical equation of spin precession (2.18). This is a manifestation of the Ehrenfest theorem, since the Hopf map (B.2) yields the expectation value of (normalised) quantum spin in the state $gu \in \mathbb{C}^2$, see [9].

Therefore, defining $\tilde{\pi}_H := \text{id}_{\mathbb{R}^d \times \mathbb{R}^d} \otimes \pi_H : \mathbb{R}^d \times \mathbb{R}^d \times \text{SU}(2) \rightarrow \mathbb{R}^d \times \mathbb{R}^d \times S^2$, i.e. $\tilde{\pi}_H(p, x, g) = (p, x, \pi_H(g))$, we obtain the following commuting diagram:

$$
\begin{array}{ccc}
(p, x, g) & \xrightarrow{Y^t} & (\Phi^t(p, x), d(p, x, t)g) \\
\downarrow \tilde{\pi}_H & & \downarrow \tilde{\pi}_H \\
(p, x, n) & \xrightarrow{Y^t_{\text{cl}}} & (\Phi^t(p, x), \varphi(d(p, x, t))n)
\end{array}
$$

Furthermore, to every (integrable) function $f \in L^1(\Omega_E \times S^2, d\mu_{\text{cl}})$ one can associate a function $F \in L^1(\Omega_E \times \text{SU}(2), d\mu)$ by defining $F := f \circ \pi_H$, i.e. $F(p, x, g) = f(p, x, \pi_H(g))$. Provided now that $Y^t$ is ergodic on $\Omega_E \times \text{SU}(2)$ with respect to $\mu = \mu_E \times \mu_H$, one observes that

$$
\lim_{T \to \infty} \frac{1}{T} \int_0^T f(Y^t_{\text{cl}}(\xi, y, \pi_H(h))) \, dt = \lim_{T \to \infty} \frac{1}{T} \int_0^T F(Y^t(\xi, y, h)) \, dt \\
= \int_{\Omega_E \times \text{SU}(2)} F(p, x, g) \, d\mu(p, x, g) \\
= \int_{\Omega_E \times S^2} f(p, x, n) \, d\mu_{\text{cl}}(p, x, n)
$$

for $\mu_E$-almost all $(\xi, y) \in \Omega_E$ and $\mu_H$-almost all $h \in \text{SU}(2)$. Since this implies the validity of (B.3) for $\mu_{S^2}$-almost $n = \pi_H(h) \in S^2$, the ergodicity of $Y^t$ implies ergodicity of $Y^t_{\text{cl}}$ on $\Omega_E \times S^2$ with respect to $\mu_{\text{cl}} = \mu_E \times \mu_{S^2}$. 

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