Semiclassics for Particles with Spin via a Wigner–Weyl-Type Calculus

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Abstract. We show how to relate the full quantum dynamics of a spin-¹/₂ particle on $\mathbb{R}^d$ to a classical Hamiltonian dynamics on the enlarged phase space $\mathbb{R}^{2d} \times \mathbb{S}^2$ up to errors of second order in the semiclassical parameter. This is done via an Egorov-type theorem for normal Wigner–Weyl calculus for $\mathbb{R}^d$ (Folland, Harmonic Analysis on Phase Space, 1989; Lein, Weyl Quantization and Semiclassics, 2010) combined with the Stratonovich–Weyl calculus for $SU(2)$ (Varilly and Gracia-Bondia, Ann Phys 190:107–148, 1989). For a specific class of Hamiltonians, including the Rabi- and Jaynes–Cummings model, we prove an Egorov theorem for times much longer than the semiclassical time scale. We illustrate the approach for a simple model of the Stern–Gerlach experiment.

1. Introduction

We consider the semiclassical limit of a quantum system with spin. The underlying state space is the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^d, \mathbb{C}^n)$ of square-integrable functions on configuration space $\mathbb{R}^d$ taking values in $\mathbb{C}^n$. The Hamiltonian $\hat{H}$ generating the time evolution on $\mathcal{H}$ is assumed to be the Weyl quantization of a matrix-valued symbol $H : \mathbb{R}^{2d} \to \mathcal{B}(\mathbb{C}^n)$, i.e.

$$\hat{H} = H\big(\varepsilon, x, -\mathrm{i}\varepsilon\nabla_x\big) := \mathrm{Op}\big(H(\varepsilon)\big).$$

Under appropriate conditions on the function H, its Weyl quantization $\hat{H}$ is a self-adjoint operator on $\mathcal{H}$ and generates a unitary group $\mathrm{e}^{-\mathrm{i}\hat{H}\frac{t}{\varepsilon}}$. We will be interested in the semiclassical asymptotics of the evolution of semiclassical observables. Let $A : \mathbb{R}^{2d} \to \mathcal{B}(\mathbb{C}^n)$ be another matrix-valued function on classical phase space, then the time evolution of the semiclassical operator $\hat{A} = \mathrm{Op}(A)$ is given by

$$\hat{A}(t) := \mathrm{e}^{+\mathrm{i}\hat{H}\frac{t}{\varepsilon}}\,\hat{A}\,\mathrm{e}^{-\mathrm{i}\hat{H}\frac{t}{\varepsilon}}$$

and $\hat{A}(t)$ solves the Heisenberg equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{A}(t) = \frac{\mathrm{i}}{\varepsilon}\left[\hat{H}, \hat{A}(t)\right].$$

Instead of solving the full quantum dynamics, one is often interested in simpler, approximate solutions in terms of a classical Hamiltonian flow. In the scalar case $n = 1$, this is the standard semiclassical problem. Under appropriate technical conditions, the Egorov Theorem states that

$$\sup_{t \in [0,T]} \left\| \hat{A}(t) - \mathrm{Op}\left(A \circ \Phi_t^0\right) \right\| = \mathcal{O}(\varepsilon), \tag{1.1}$$

where $\Phi_t^0 : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ denotes the classical Hamiltonian flow corresponding to the principal symbol $H_0(q,p)$ of $H(q,p) = H_0(q,p) + \mathcal{O}(\varepsilon)$. That is, on bounded time intervals, one can approximate the quantum mechanical time evolution of a semiclassical observable by transporting its symbol along a Hamiltonian flow. As a corollary, the Egorov theorem also implies a semiclassical evolution for states: here, the Wigner transform of the time-evolved density operator is compared to the Wigner transform of the density operator at $t = 0$ transported in time using the classical flow. In addition to its physical and practical relevance for understanding the quantum time evolution, the Egorov theorem is also the basis for a number of further mathematical results connecting properties of quantum and classical systems. For example, in [1,25] quantum ergodicity for classically ergodic systems was proved based on the Egorov theorem.

The result (1.1) has been generalized in many directions. For example, when replacing the flow Φ_t^0 by the flow Φ_t^ε generated by $H_0(q,p) + \varepsilon H_1(q,p)$, where $H(q,p) = H_0(q,p) + \varepsilon H_1(q,p) + \mathcal{O}(\varepsilon^2)$, then the error is of order ε^2,

$$\sup_{t \in [0,T]} \left\| \hat{A}(t) - \mathrm{Op}\left(A \circ \Phi_t^\varepsilon\right) \right\| = \mathcal{O}(\varepsilon^2). \tag{1.2}$$

It is also well known how to construct higher order approximations to $\hat{A}(t)$. However, they cannot be written as the composition of A with a flow map on phase space $\mathbb{R}^{2d}$, see e.g. [18, Chaptre IV §6]. Depending on the details of the classical flow, one can potentially extend this approximation to longer time scales [3,5].

In this work, we consider the case $n > 1$ of matrix-valued symbols. Then, basically two distinct cases appear: If the principal symbol H_0 of H has eigen spaces that are non-trivial functions on $\mathbb{R}^{2d}$, then this is an adiabatic problem. Hence, in a first step, the total state space $\mathcal{H} = L^2(\mathbb{R}^d, \mathbb{C}^n)$ of the system can be decomposed into orthogonal subspaces $\mathcal{H}_j$ that are each unitarily equivalent to spaces of the form $L^2(\mathbb{R}^d, \mathbb{C}^{n_j})$ with $\sum_j n_j = n$, see [7,14,16,17,19]. The operator $\hat{H}$ is then block-diagonal with respect to these subspaces up to errors of order ε^∞ and thus the reduced problems on each $L^2(\mathbb{R}^d, \mathbb{C}^{n_j})$ can be analyzed independently. If a subspace $\mathcal{H}_j$ is related to an isolated eigenvalue band E_j of the principal symbol H_0, i.e. $E_j(q,p)$ depends smoothly on (q,p) and is an eigenvalue of $H_0(q,p)$ with constant multiplicity, then the block of

$\hat{H}$ on that subspace is unitarily equivalent to a semiclassical Hamiltonian $\hat{H}_j$ on $L^2(\mathbb{R}^d, \mathbb{C}^{n_j})$ with principal symbol $E_j \mathbf{1}_{\mathbb{C}^{n_j}}$ where $\mathbf{1}_{\mathbb{C}^{n_j}} = \mathrm{diag}(1, \ldots, 1)$.

These semiclassical Hamiltonians $H_j \simeq E_j \mathbf{1}_{\mathbb{C}^{n_j}} + \mathcal{O}(\varepsilon)$ are an example for the type of Hamiltonian we will study in this paper: here, the principal symbol H_0 is a scalar multiple of the identity matrix. Since higher order terms do not contribute on the time scales we are interested in, we assume in the following that the symbol of the Hamiltonian has the form

$$H(q,p) = H_0(q,p) + \varepsilon\, H_1(q,p) = h_0(q,p)\, \mathbf{1}_{\mathbb{C}^n} + \varepsilon\, H_1(q,p).$$

Also, the semiclassical limit for this problem has been studied extensively in the literature, see e.g. [1] and references therein. However, the fact that A is matrix-valued and that the quantum dynamics is non-trivial on the spin degrees of freedom makes it impossible to approximate $\hat{A}(t)$ in terms of a classical flow only on $\mathbb{R}^{2d}$ as in (1.1) or (1.2). Instead it is shown in [1] based on [4] that the symbol of $\hat{A}(t)$ can be approximated, to leading order, by

$$A(t,q,p) = D^*(t,q,p)\, \big(A \circ \Phi_t^0\big)(q,p)\, D(t,q,p), \qquad (1.3)$$

where Φ_t^0 is the Hamiltonian flow of the scalar principal symbol $h_0(q,p)$ of H. The orthogonal matrices $D(t,q,p)$ are generated by the sub-principal symbol H_1 according to

$$\frac{\mathrm{d}}{\mathrm{d}t} D(t,q,p) = -\mathrm{i}\,\big(H_1 \circ \Phi_t^0\big)(q,p)\, D(t,q,p), \qquad D(0,q,p) = \mathbf{1}_{\mathbb{C}^n}.$$

From the point of view of our results, this description has two shortcomings: it gives only a leading order description, i.e. an error term as in (1.1), and the time-evolved $A(t,q,p)$ is not given in terms of a flow on phase space.

The latter shortcoming was solved in [2], where the authors observed that one can use a Weyl calculus for spin developed by Stratonovich [20] and further elaborated upon by Gracia-Bondìa and Vàrilly [23] to map matrix-valued functions A on $\mathbb{R}^{2d}$ to scalar functions $a := \mathrm{Symb}_{\mathbb{S}^2}(A)$ on the *extended phase space* $\Sigma := \mathbb{R}^{2d} \times \mathbb{S}^2$. Note that the two-sphere $\mathbb{S}^2$ carries a natural symplectic form, namely the volume form. The result is that $A(t,q,p)$ as in (1.3) can indeed be written in terms of a so-called skew-product flow Φ_t^{skew} on $\mathbb{R}^{2d} \times \mathbb{S}^2$,

$$\mathrm{Symb}_{\mathbb{S}^2}\big(A(t,q,p)\big) =: a(t,q,p,n) = \big(a \circ \Phi_t^{\mathrm{skew}}\big)(q,p,n).$$

Note that the skew-product flow Φ_t^{skew} is not a Hamiltonian flow and that the initial "spin" n has no effect on the dynamics of the translational degrees of freedom, i.e. with $\Phi_t^{\mathrm{skew}} =: \big(Q_t^{\mathrm{skew}}, P_t^{\mathrm{skew}}, N_t^{\mathrm{skew}}\big)$ it holds that $Q_t^{\mathrm{skew}}(q,p,n) = Q_t^{\mathrm{skew}}(q,p)$ and $P_t^{\mathrm{skew}}(q,p,n) = P_t^{\mathrm{skew}}(q,p)$ are both independent of n. This is somewhat unsatisfactory from a physical point of view, since the paradigmatic experiment measuring the spin of a particle, the Stern–Gerlach experiment, is based on the fact that the trajectory of a particle with spin in an inhomogeneous magnetic field depends on its spin orientation. However, this is a small effect not seen in the leading-order approximation.

The main new result of the present paper is the construction of a *Hamiltonian* flow Φ_t^ε on the extended phase space $\Sigma = \mathbb{R}^{2d} \times \mathbb{S}^2$ that *includes the*

influence of spin on the translational degrees of freedom and provides a better approximation to the evolution of scalar observables $A = a\,\mathbf{1}_{\mathbb{C}^n}$,

$$\sup_{t\in[0,T]} \left\| \hat{A}(t) - \mathrm{Op}_\Sigma\left(a \circ \Phi_t^\varepsilon\right) \right\| = \mathcal{O}(\varepsilon^2). \tag{1.4}$$

Here, Op_Σ denotes the quantization map from functions on Σ to operators on $L^2(\mathbb{R}^{2d}, \mathbb{C}^n)$ and $a(q, p, n) := a(q, p)$ (cf. Sect. 2 for details).

For a special class of Hamiltonians on $L^2(\mathbb{R}, \mathbb{C}^2)$, including the Rabi and the Jaynes–Cummings models, we show that the above approximation remains valid for longer times: Assume $h_0(q, p) = \frac{1}{2}(p^2 + \omega^2 q^2)$ is the one-dimensional harmonic oscillator Hamiltonian and suppose that the entries of $H_1(q, p)$ are polynomials in q and p of degree at most one. Then, we can prove (1.4) for longer times at the expense of a larger error. More precisely, we arrive at the estimate

$$\sup_{t\in[0,T/\varepsilon^\gamma]} \left\| \hat{A}(t) - \mathrm{Op}_\Sigma\left(a \circ \Phi_t^\varepsilon\right) \right\| = \mathcal{O}(\varepsilon^{3/2-3\gamma}) \tag{1.5}$$

for any $0 \leq \gamma < 1/2$. Note that, on this time scale, the influence of spin on the position of the particle can be of order $\varepsilon^{1-2\gamma}$, so almost of order 1. Moreover, even for general initial observables $\hat{B} = \mathrm{Op}_\Sigma(b)$ with $b = b(q, p, n)$ depending also on spin, we can go to slightly longer times and show that

$$\sup_{t\in[0,T/\varepsilon^\gamma]} \left\| \hat{B}(t) - \mathrm{Op}_\Sigma\left(b \circ \Phi_t^\varepsilon\right) \right\| = \mathcal{O}(\varepsilon^{1-4\gamma}) \tag{1.6}$$

holds for any $0 \leq \gamma < 1/4$. Concrete applications of these results to the Rabi and the Jaynes–Cummings model are discussed elsewhere [11]. Note that without spin the semiclassical approximation for the harmonic oscillator h_0 is exact. On the extended phase-space $\mathbb{R}^2 \times \mathbb{S}^2$ this is no longer true, even when h_1 is linear in q and p. However, in Theorem 3.4, we show that there is still an exact evolution equation for the symbol $a(t)$ of $\hat{A}(t)$. But this equation can no longer be solved by classical transport.

The paper is organized as follows: In Sect. 2, we first recall the standard Weyl calculus on $\mathbb{R}^{2d}$, then introduce the Stratonovich–Weyl calculus on $\mathbb{S}^2$ and finally show how to combine them. While this idea is not new (e.g. [2,22]), the results of Sect. 2.3 have not been worked out in this form before. Section 3 contains the rigorous statements and the proofs of the general and the long-time Egorov theorems. Their proofs rely on estimates on the derivatives of the classical flow on Σ which we show in Sect. 4. In the final Sect. 5, we illustrate the method by applying it to a simple model for the Stern–Gerlach experiment. We conclude, in particular, that the semiclassical approximation captures the spin-dependent splitting of wave packets correctly.

2. Weyl Calculus

2.1. Standard Weyl Calculus on $\mathbb{R}^{2d}$

We briefly recall the most important features of Weyl calculus and specific properties that we will use in the following. Readers familiar with Weyl calculus

and not interested in the mathematical technicalities can skip this section. For more details on ε-pseudodifferential operators, we refer e.g. to [12,15,21]. For a short summary on Weyl calculus with operator-valued symbols, the readers can also consult Appendix A of [22].

One common and well-studied class of pseudodifferential operators are those which are Weyl quantizations of symbols. A *symbol f of order $k \in \mathbb{R}$* is a smooth function from $\mathbb{R}^{2d}$ to $\mathcal{B}(\mathbb{C}^n)$ such that

$$\|f\|_{k,r} := \max_{\substack{\alpha,\beta \in \mathbb{N}_0^d \\ |\alpha|+|\beta| \leq r}} \sup_{(q,p) \in \mathbb{R}^{2d}} \left\| \langle p \rangle^{-k+|\alpha|} \partial_p^\alpha \partial_q^\beta f(q,p) \right\|_{\mathcal{B}(\mathbb{C}^n)}$$

is bounded for all $r \in \mathbb{N}_0$. Here, $\langle p \rangle^k := (1+|p|^2)^{k/2}$. Equipped with the family of seminorms $\{\|\cdot\|_{k,r}\}_{r \in \mathbb{N}_0}$, the set of all symbols of order k, denoted with S^k, is a Fréchet space. Functions in S^k have the property, that derivatives with respect to p improve the decay with respect to p. In particular, any partial derivative of degree k with respect to p of a function in S^k yields a bounded function with bounded derivatives. The space of uniformly bounded functions $A : [0,\varepsilon_0] \longrightarrow S^k$ is denoted by $S^k(\varepsilon)$.

For a Schwartz function $\psi \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^n)$ and $A \in S^k(\varepsilon)$, the action of the Weyl quantization $\hat{A} = \mathrm{Op}_{\mathbb{R}^{2d}}(A)$ of A can be defined through the oscillatory integral

$$
\begin{aligned}
(\hat{A}\psi)(x) &= \big(\mathrm{Op}_{\mathbb{R}^{2d}}(A)\psi\big)(x) \\
&= \frac{1}{(2\pi\varepsilon)^d} \int\limits_{\mathbb{R}^{2d}} \mathrm{d}p \, \mathrm{d}y \, A\big(\varepsilon, \tfrac{1}{2}(x+y), p\big) \, \mathrm{e}^{+\frac{\mathrm{i}}{\varepsilon} p \cdot (x-y)} \, \psi(y).
\end{aligned}
\tag{2.1}
$$

For $k \leq 0$, by the Caldéron–Vaillancourt theorem [18, Thorme II 36], $\hat{A}$ can be extended to a bounded operator on $\mathcal{H} = L^2(\mathbb{R}^d, \mathbb{C}^n)$; we will discuss other boundedness criteria in Sect. 3.

The inverse of Op is the Wigner transform: if K_A is the operator kernel to $\hat{A} \in \mathcal{B}(L^2(\mathbb{R}^d, \mathbb{C}^n))$, then we define

$$\big(\mathcal{W}_{\mathbb{R}^{2d}}(\hat{A})\big)(q,p) := \frac{1}{(2\pi)^{d/2}} \int\limits_{\mathbb{R}^d} \mathrm{d}y \, \mathrm{e}^{-\mathrm{i}y \cdot p} \, K_A\big(q + \tfrac{\varepsilon}{2}y, q - \tfrac{\varepsilon}{2}y\big).$$

The composition of operators induces a composition of symbols. For any $A \in S^{k_1}(\varepsilon)$ and $B \in S^{k_2}(\varepsilon)$, there exists a symbol $C \in S^{k_1+k_2}(\varepsilon)$ denoted by $C = A \# B$ such that $\hat{A}\hat{B} = \hat{C}$. The bilinear map $\# : S^{k_1} \times S^{k_2} \to S^{k_1+k_2}$ is called the Moyal product and it is continuous with respect to the Frèchet topologies uniformly in ε, i.e. for any $r \in \mathbb{N}_0$ there is a $\tilde{r} \in \mathbb{N}_0$ and a constant $c_{r,\tilde{r}} < \infty$ such that

$$\big\|(A\#B)(\varepsilon)\big\|_{k_1+k_2,r} \leq c_{r,\tilde{r}} \big\|A(\varepsilon)\big\|_{k_1,\tilde{r}} \big\|B(\varepsilon)\big\|_{k_2,\tilde{r}}$$

holds true for all $\varepsilon \in [0,\varepsilon_0]$. The last statement follows e.g. from inspecting the proof of Thm. 2.41 in [9]. If for $A \in S^k(\varepsilon)$ there exists a sequence $(A_j)_{j \in \mathbb{N}_0}$ in $S^k(\varepsilon)$ such that

$$\sup_{\varepsilon \in [0,\varepsilon_0)} \left\| \varepsilon^{-(m+1)} \left(A(\varepsilon) - \sum_{j=0}^{m} \varepsilon^j A_j(\varepsilon) \right) \right\|_{k,r} < \infty$$

for all $r \in \mathbb{N}_0$ and $m \in \mathbb{N}_0$, then one writes $A \asymp \sum_{j=0}^{\infty} \varepsilon^j A_j$ in $S^k(\varepsilon)$. If $A \in S^k(\varepsilon)$ has an asymptotic expansion with coefficients $A_j \in S^{k-j}$ not depending on ε, then A is called a classical symbol, A_0 its principal symbol and A_1 its subprincipal symbol. The Moyal product $C := A \# B \in S^{k_1+k_2}(\varepsilon)$ of symbols $A \in S^{k_1}(\varepsilon)$ and $B \in S^{k_2}(\varepsilon)$ has an explicit asymptotic expansion $C \asymp \sum_{j=0}^{\infty} \varepsilon^j C_j$ such that $C_j \in S^{k_1+k_2-j}(\varepsilon)$ and the remainder maps

$$R_{m+1} : S^{k_1} \times S^{k_2} \to S^{k_1+k_2-m-1} \,,$$

$$(A, B) \mapsto R_{m+1} := \varepsilon^{-(m+1)} \left(C(\varepsilon) - \sum_{j=0}^{m} \varepsilon^j C_j(\varepsilon) \right)$$

are continuous. The expansion starts with the pointwise product $C_0(\varepsilon) = A(\varepsilon)B(\varepsilon)$ and the Poisson bracket $C_1(\varepsilon) = -\frac{i}{2}\{A(\varepsilon), B(\varepsilon)\}_{\mathbb{R}^{2d}}$, where

$$\{A, B\}_{\mathbb{R}^{2d}} := \nabla_p A \cdot \nabla_q B - \nabla_q A \cdot \nabla_p B := \sum_{j=1}^{d} \left(\partial_{p_j} A \, \partial_{q_j} B - \partial_{q_j} A \, \partial_{p_j} B \right).$$

For classical symbols A and B, the Moyal product $C := A \# B$ is also a classical symbol with an asymptotic expansion starting with

$$A \# B \asymp A_0 B_0 + \varepsilon \left(A_1 B_0 + A_0 B_1 - \tfrac{i}{2}\{A_0, B_0\}_{\mathbb{R}^{2d}} \right) + \mathcal{O}(\varepsilon^2).$$

If $A = a \, \mathbf{1}_{\mathbb{C}^n}$ is a scalar multiple of the identity, then A and all its derivatives commute pointwise with any B. As a consequence, one can show that in this case

$$[A_0, B_0]_\sharp := A_0 \# B_0 - B_0 \# A_0 \asymp -i\varepsilon\{A_0, B_0\}_{\mathbb{R}^{2d}} + \mathcal{O}(\varepsilon^3). \qquad (2.2)$$

The fact that the remainder term in (2.2) is of order ε^3 and not only ε^2 is at the basis of our higher order semiclassical approximations. It distinguishes Weyl quantization from other quantization rules.

2.2. Stratonovich–Weyl Calculus for Spin

Similar to Weyl calculus that maps functions on phase space $\mathbb{R}^{2d}$ to operators on the Hilbert space $L^2(\mathbb{R}^d)$, there is a Weyl calculus that associates functions on the compact phase space $\mathbb{S}^2$ to operators on the finite-dimensional Hilbert spaces $\mathbb{C}^n$. It was first proposed by Stratonovich [20] and elaborated upon further by Gracia-Bondia and Varilly [23,24], and has been applied to study the dynamics at Josephson junctions [6].

To make the following as transparent as possible, we restrict the presentation to the case of $\mathbb{C}^2$ and use the letter n to denote a point on the unit sphere $\mathbb{S}^2$ from now on. Higher dimensional spin-spaces can be dealt with in complete analogy [23,24]. The basic observation is that any 2×2 matrix can

be written as a linear combination of the identity matrix $\mathbf{1}_{\mathbb{C}^2}$ and the three Pauli matrices σ_j, $j = 1, 2, 3$,

$$A = \mathfrak{a}_0 \, \mathbf{1}_{\mathbb{C}^2} + \sum_{j=1}^{3} \mathfrak{a}_j \, \sigma_j = \mathfrak{a}_0 \, \mathbf{1}_{\mathbb{C}^2} + \mathfrak{a} \cdot \sigma \tag{2.3}$$

for some complex coefficients $\mathfrak{a}_0, \ldots, \mathfrak{a}_3 \in \mathbb{C}$. Now, the quantization map $\mathrm{Op}_{\mathbb{S}^2} : C^\infty(\mathbb{S}^2) \to \mathcal{B}(\mathbb{C}^2)$ can be defined most easily using the *Stratonovich–Weyl kernel*

$$\Delta(n) := \tfrac{1}{2}\big(\mathbf{1}_{\mathbb{C}^2} + \sqrt{3}\, n \cdot \sigma\big), \quad n \in \mathbb{S}^2, \tag{2.4}$$

by setting

$$\mathrm{Op}_{\mathbb{S}^2}(a) := \frac{1}{2\pi} \int_{\mathbb{S}^2} dn \, a(n)\, \Delta(n). \tag{2.5}$$

It is clearly many to one, but there is a natural way to define also a dequantization map $\mathcal{W}_{\mathbb{S}^2} : \mathcal{B}(\mathbb{C}^2) \to C^\infty(\mathbb{S}^2)$ by

$$\big(\mathcal{W}_{\mathbb{S}^2}(A)\big)(n) := \mathrm{Tr}_{\mathbb{C}^2}\big(A\, \Delta(n)\big). \tag{2.6}$$

which maps onto the four-dimensional subspace $C_1(\mathbb{S}^2) := \mathrm{span}\{1, n_1, n_2, n_3\}$ of $C^\infty(\mathbb{S}^2)$. Using $\mathrm{Tr}_{\mathbb{C}^2} \sigma_j = 0$, we find that the dequantization of A written as in (2.3) is the linear polynomial

$$a(n) = \big(\mathcal{W}_{\mathbb{S}^2}(A)\big)(n) = \mathfrak{a}_0 + \sqrt{3}\, \mathfrak{a} \cdot n, \tag{2.7}$$

and $\mathrm{Op}_{\mathbb{S}^2} : C_1(\mathbb{S}^2) \to \mathcal{B}(\mathbb{C}^2)$ is indeed one-to-one with inverse $\mathcal{W}_{\mathbb{S}^2}$. The projection $\mathcal{P} = \mathcal{W}_{\mathbb{S}^2} \circ \mathrm{Op}_{\mathbb{S}^2}$ maps any $a \in C^\infty(\mathbb{S}^2)$ to the representative in $C_1(\mathbb{S}^2)$ that quantizes to the same matrix and is explicitly given by

$$(\mathcal{P}a)(n) = \frac{1}{2\pi} \int_{\mathbb{S}^2} dk \, a(k)\, \mathrm{Tr}_{\mathbb{C}^2}\big(\Delta(k)\, \Delta(n)\big) = \frac{1}{4\pi} \int_{\mathbb{S}^2} dk \, a(k) \big(1 + 3k \cdot n\big)$$

$$= \frac{1}{4\pi} \int_{\mathbb{S}^2} dk \, a(k) + \sqrt{3}\, \left(\frac{\sqrt{3}}{4\pi} \int_{\mathbb{S}^2} dk \, k \, a(k)\right) \cdot n$$

$$=: \mathfrak{a}_0 + \sqrt{3}\, \mathfrak{a} \cdot n \tag{2.8}$$

For later reference we note that for all $a \in C^\infty(\mathbb{S}^2)$ we have that

$$\mathcal{P}a = a \qquad \text{for all } a \in C_1(\mathbb{S}^2) \tag{2.9}$$

$$\mathrm{Op}_{\mathbb{S}^2} \mathcal{P}a = \mathrm{Op}_{\mathbb{S}^2} a \quad \text{for all } a \in C^\infty(\mathbb{S}^2). \tag{2.10}$$

Since the symbol a of a given matrix A is not unique, there is a priori also no unique way to define the corresponding Moyal product $\sharp_{\mathbb{S}^2}$, i.e. the matrix product on the level of functions on $\mathbb{S}^2$. However, if we demand that it takes

its values in $C_1(\mathbb{S}^2)$, it is unique and one finds

$$
\begin{aligned}
(a \,\sharp_{\mathbb{S}^2} b)(n) &:= \mathcal{W}_{\mathbb{S}^2}\left(\mathrm{Op}_{\mathbb{S}^2}(a)\,\mathrm{Op}_{\mathbb{S}^2}(b)\right) = \mathcal{W}_{\mathbb{S}^2}\left(\mathrm{Op}_{\mathbb{S}^2}(\mathcal{P}a)\,\mathrm{Op}_{\mathbb{S}^2}(\mathcal{P}b)\right) \\
&= \mathcal{W}_{\mathbb{S}^2}\left((\mathfrak{a}_0\,\mathbf{1}_{\mathbb{C}^2} + \mathfrak{a}\cdot\sigma)(\mathfrak{b}_0\,\mathbf{1}_{\mathbb{C}^2} + \mathfrak{b}\cdot\sigma)\right) \\
&= \mathcal{W}_{\mathbb{S}^2}\left((\mathfrak{a}_0\mathfrak{b}_0 + \mathfrak{a}\cdot\mathfrak{b}) + (\mathfrak{a}_0\mathfrak{b} + \mathfrak{a}\mathfrak{b}_0 + \mathrm{i}\,\mathfrak{a}\wedge\mathfrak{b})\cdot\sigma\right) \\
&= (\mathfrak{a}_0\mathfrak{b}_0 + \mathfrak{a}\cdot\mathfrak{b}) + \sqrt{3}\left(\mathfrak{a}_0\mathfrak{b} + \mathfrak{a}\mathfrak{b}_0 + \mathrm{i}\,\mathfrak{a}\wedge\mathfrak{b}\right)\cdot n. \qquad (2.11)
\end{aligned}
$$

As for the calculus on $\mathbb{R}^{2d}$, the applicability to the semiclassical limit of the Heisenberg equations of motion rests on the observation that the commutator of operators corresponds to the Poisson bracket of symbols. The natural symplectic form on $\mathbb{S}^2$ is the volume form η, which we normalize such that for two tangent vectors v, w at $n \in \mathbb{S}^2$

$$
\eta_n(v, w) = -\tfrac{\sqrt{3}}{2}(v \wedge w)\cdot n.
$$

Thus, the Hamiltonian vector field associated to a function $a \in C^\infty(\mathbb{S}^2)$ is

$$
X^a = -\tfrac{2}{\sqrt{3}}\,\nabla_n a \wedge n
$$

and a short computation yields

$$
\{a, b\}_{\mathbb{S}^2} := \eta\left(X^a, X^b\right) = -\tfrac{2}{\sqrt{3}}\left(\nabla_n a \wedge \nabla_n b\right)\cdot n.
$$

Comparing with (2.11), we immediately see that

$$
[a, b]_{\sharp_{\mathbb{S}^2}} := a \,\sharp_{\mathbb{S}^2} b - b \,\sharp_{\mathbb{S}^2} a = -\mathrm{i}\,\{\mathcal{P}a, \mathcal{P}b\}_{\mathbb{S}^2}. \qquad (2.12)
$$

Now, there is an observation which is crucial for the following:

Lemma 2.1. *Let* $a, b \in C^\infty(\mathbb{S}^2)$, *then*

$$
\{\mathcal{P}a, \mathcal{P}b\}_{\mathbb{S}^2} = \mathcal{P}\,\{\mathcal{P}a, b\}_{\mathbb{S}^2}. \qquad (2.13)
$$

Proof. We write $(\mathcal{P}a)(n) = \mathfrak{a}_0 + \sqrt{3}\,\mathfrak{a}\cdot n$ and $(\mathcal{P}b)(n) = \mathfrak{b}_0 + \sqrt{3}\,\mathfrak{b}\cdot n$. Then,

$$
\begin{aligned}
\mathcal{P}\,\{\mathcal{P}a, b\}_{\mathbb{S}^2} = &-\frac{2}{4\pi}\int_{\mathbb{S}^2} \mathrm{d}k\,(\mathfrak{a}\wedge\nabla_n b(k))\cdot k \\
&-\sqrt{3}\left(\frac{2\sqrt{3}}{4\pi}\int_{\mathbb{S}^2}\mathrm{d}k\,k\,(\mathfrak{a}\wedge\nabla_n b(k))\cdot k\right)\cdot n.
\end{aligned}
$$

Integration by parts gives for the first term

$$
\int_{\mathbb{S}^2}\mathrm{d}k\,(\mathfrak{a}\wedge\nabla_n b)\cdot k = \int_{\mathbb{S}^2}\mathrm{d}k\,\epsilon_{jlm}\,\mathfrak{a}_j\,\partial_l b(k)\,k_m = 0
$$

and for the jth component of the second term

$$\int_{\mathbb{S}^2} \mathrm{d}k \, k_j \left(\mathfrak{a} \wedge \nabla_n b(k) \right) \cdot k = \int_{\mathbb{S}^2} \mathrm{d}k \, k_j \, \epsilon_{lms} \, \mathfrak{a}_l \, \partial_m b(k) \, k_s$$

$$= -\int_{\mathbb{S}^2} \mathrm{d}k \, \epsilon_{ljs} \, \mathfrak{a}_l \, b(k) \, k_s = -\epsilon_{jsl} \, \mathfrak{a}_l \int_{\mathbb{S}^2} \mathrm{d}k \, b(k) \, k_s$$

$$= (\mathfrak{a} \wedge \mathfrak{b})_j \, \frac{4\pi}{\sqrt{3}}.$$

Comparing with $\{\mathcal{P}a, \mathcal{P}b\}_{\mathbb{S}^2} = -2\sqrt{3}(\mathfrak{a} \wedge \mathfrak{b}) \cdot n$ proves the claim.　　　□

Corollary 2.2. *Let $a \in C_1(\mathbb{S}^2)$ and $b \in C^\infty(\mathbb{S}^2)$. Then,*

$$\left[\mathrm{Op}_{\mathbb{S}^2} a, \mathrm{Op}_{\mathbb{S}^2} b \right] = -\mathrm{i} \, \mathrm{Op}_{\mathbb{S}^2} \{a, b\}_{\mathbb{S}^2}. \qquad (2.14)$$

Proof.

$$\left[\mathrm{Op}_{\mathbb{S}^2} a, \mathrm{Op}_{\mathbb{S}^2} b \right] = \mathrm{Op}_{\mathbb{S}^2} [a, b]_{\sharp_{\mathbb{S}^2}} \overset{(2.12)}{=} -\mathrm{i} \, \mathrm{Op}_{\mathbb{S}^2} \{\mathcal{P}a, \mathcal{P}b\}_{\mathbb{S}^2}$$

$$\overset{(2.13)}{=} -\mathrm{i} \, \mathrm{Op}_{\mathbb{S}^2} \mathcal{P} \{\mathcal{P}a, b\}_{\mathbb{S}^2} \overset{(2.10)}{=} -\mathrm{i} \, \mathrm{Op}_{\mathbb{S}^2} \{\mathcal{P}a, b\}_{\mathbb{S}^2}$$

$$\overset{(2.9)}{=} -\mathrm{i} \, \mathrm{Op}_{\mathbb{S}^2} \{a, b\}_{\mathbb{S}^2}.$$

　　　□

2.3. Weyl Calculus on $\mathbb{R}^{2d} \times \mathbb{S}^2$

It is now straightforward to define a Weyl calculus on the product $\Sigma = \mathbb{R}^{2d} \times \mathbb{S}^2$. We say $a \in S_\Sigma^k(\varepsilon)$, if $a(\varepsilon) \in C^\infty(\Sigma)$ such that $\mathrm{Op}_{\mathbb{S}^2} a \in S^k(\varepsilon)$. For $a \in S_\Sigma^k(\varepsilon)$, define Op_Σ and $\mathcal{W}_\Sigma$ by

$$\mathrm{Op}_\Sigma(a) := \mathrm{Op}_{\mathbb{R}^{2d}} \left(\mathrm{Op}_{\mathbb{S}^2}(a) \right),$$

$$\mathcal{W}_\Sigma(\hat{A}) := \mathcal{W}_{\mathbb{R}^{2d}} \left(\mathcal{W}_{\mathbb{S}^2}(\hat{A}) \right),$$

and let

$$\{a, b\}_\Sigma := \{a, b\}_{\mathbb{R}^{2d}} + \tfrac{1}{\varepsilon} \{a, b\}_{\mathbb{S}^2}.$$

We now formulate our assumptions on the symbol of the Hamiltonian.

Assumption 2.3. *Let $h(q, p, n) = h_0(q, p) + \varepsilon \, h_1(q, p, n)$ such that $h_0 \in S^2$ and*

$$h_1(q, p, n) = \mathfrak{h}_0(q, p) + \sqrt{3} \, \mathfrak{h}(q, p) \cdot n$$

with $\mathfrak{h}_0$ and all components of $\mathfrak{h}(q, p)$ in S^1.

　　　Note that in view of (2.8) and (2.10), assuming h is a linear polynomial in n is not a restriction, merely a convenient way to write the symbol.

Lemma 2.4. *Let h satisfies Assumption 2.3 and let $a \in S_\Sigma^0(\varepsilon)$.*

(i)　*Then,*

$$\left\| \frac{\mathrm{i}}{\varepsilon} \left[\mathrm{Op}_\Sigma h, \mathrm{Op}_\Sigma a \right] - \mathrm{Op}_\Sigma \{h, a\}_\Sigma \right\|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}(\varepsilon).$$

(ii)　*If, in addition, there is a symbol a_0 such that $a(q, p, n) - a_0(q, p) = \mathcal{O}(\varepsilon)$, then*

$$\left\| \frac{\mathrm{i}}{\varepsilon} \big[\mathrm{Op}_\Sigma h \,, \mathrm{Op}_\Sigma a \big] - \mathrm{Op}_\Sigma \{h, a\}_\Sigma \right\|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}(\varepsilon^2).$$

(iii)   *Suppose that h_0 is a quadratic polynomial in the components of p and q, and the components of $\mathfrak{h}_0$ and $\mathfrak{h}$ are linear polynomials in q and p. Then,*

$$\frac{\mathrm{i}}{\varepsilon} \big[\mathrm{Op}_\Sigma h, \mathrm{Op}_\Sigma a \big] = \mathrm{Op}_\Sigma \{h, a\}_\Sigma + \tfrac{\varepsilon}{2} \mathrm{Op}_{\mathbb{R}^{2d}} \Big(\{H_1, A\}_{\mathbb{R}^{2d}} - \{A, H_1\}_{\mathbb{R}^{2d}}$$
$$- 2\, \mathrm{Op}_{\mathbb{S}^2} \{h_1, a\}_{\mathbb{R}^{2d}} \Big)$$
$$= \mathrm{Op}_\Sigma \{h, a\}_\Sigma - \tfrac{\varepsilon}{2} \mathrm{Op}_\Sigma \{ h_1, (1 - \mathcal{P})a \}_{\mathbb{R}^{2d}}$$

holds true where $H_1 = \mathrm{Op}_{\mathbb{S}^2} h_1$ and $A = \mathrm{Op}_{\mathbb{S}^2} a$.

The main ingredient in the proof of (iii) is the following auxiliary

Lemma 2.5. *Let $a, b \in C^\infty(\Sigma)$ such that $a(q, p, \cdot), b(q, p, \cdot) \in C_1(\mathbb{S}^2)$ are at most linear polynomials in n for all $(q, p) \in \mathbb{R}^{2d}$. Then,*

$$R(a, b) := \{\mathrm{Op}_{\mathbb{S}^2} a, \mathrm{Op}_{\mathbb{S}^2} b\}_{\mathbb{R}^{2d}} - \{\mathrm{Op}_{\mathbb{S}^2} b, \mathrm{Op}_{\mathbb{S}^2} a\}_{\mathbb{R}^{2d}} - 2\, \mathrm{Op}_{\mathbb{S}^2} \{a, b\}_{\mathbb{R}^{2d}} = 0.$$

Proof of Lemma 2.4.   (i)   For the scalar symbol $h_0 \in S^2$, we have according to (2.2)

$$\big[\mathrm{Op}_{\mathbb{S}^2} h_0 \,, \mathrm{Op}_{\mathbb{S}^2} a \big]_\sharp = -\mathrm{i}\,\varepsilon \{ \mathrm{Op}_{\mathbb{S}^2} h_0, \mathrm{Op}_{\mathbb{S}^2} a \}_{\mathbb{R}^{2d}} + \mathcal{O}(\varepsilon^3), \qquad (2.15)$$

where the remainder is order ε^3 in $S^{-1}(\varepsilon)$. For h_1,

$$\big[\mathrm{Op}_{\mathbb{S}^2} h_1 \,, \mathrm{Op}_{\mathbb{S}^2} a \big]_\sharp = \big[\mathrm{Op}_{\mathbb{S}^2} h_1, \mathrm{Op}_{\mathbb{S}^2} a \big]$$
$$- \varepsilon \frac{\mathrm{i}}{2} \Big(\{ \mathrm{Op}_{\mathbb{S}^2} h_1, \mathrm{Op}_{\mathbb{S}^2} a \}_{\mathbb{R}^{2d}} - \{ \mathrm{Op}_{\mathbb{S}^2} a, \mathrm{Op}_{\mathbb{S}^2} h_1 \}_{\mathbb{R}^{2d}} \Big) + \mathcal{O}(\varepsilon^2) \qquad (2.16)$$

where the remainder is order ε^2 in $S^{-1}(\varepsilon)$. Hence,

$$\frac{\mathrm{i}}{\varepsilon} \big[\mathrm{Op}_\Sigma h \,, \mathrm{Op}_\Sigma a \big] = \mathrm{Op}_{\mathbb{R}^{2d}} \Big(\{ \mathrm{Op}_{\mathbb{S}^2} h_0, \mathrm{Op}_{\mathbb{S}^2} a \}_{\mathbb{R}^{2d}} + \mathrm{i} \big[\mathrm{Op}_{\mathbb{S}^2} h_1, \mathrm{Op}_{\mathbb{S}^2} a \big]$$
$$+ \frac{\varepsilon}{2} \Big(\{ \mathrm{Op}_{\mathbb{S}^2} h_1, \mathrm{Op}_{\mathbb{S}^2} a \}_{\mathbb{R}^{2d}} - \{ \mathrm{Op}_{\mathbb{S}^2} a, \mathrm{Op}_{\mathbb{S}^2} h_1 \}_{\mathbb{R}^{2d}} \Big) \Big) + \mathcal{O}(\varepsilon^2),$$
$$\overset{(2.14)}{=} \mathrm{Op}_{\mathbb{R}^{2d}} \Big(\mathrm{Op}_{\mathbb{S}^2} \{h_0, a\}_{\mathbb{R}^{2d}} + \mathrm{Op}_{\mathbb{S}^2} \{h_1, a\}_{\mathbb{S}^2}$$
$$+ \varepsilon\, \mathrm{Op}_{\mathbb{S}^2} \{h_1, a\}_{\mathbb{R}^{2d}} + \frac{\varepsilon}{2} \Big(\{ \mathrm{Op}_{\mathbb{S}^2} h_1, \mathrm{Op}_{\mathbb{S}^2} a \}_{\mathbb{R}^{2d}}$$
$$- \{ \mathrm{Op}_{\mathbb{S}^2} a, \mathrm{Op}_{\mathbb{S}^2} h_1 \}_{\mathbb{R}^{2d}} - 2\, \mathrm{Op}_{\mathbb{S}^2} \{h_1, a\}_{\mathbb{R}^{2d}} \Big) \Big) + \mathcal{O}(\varepsilon^2)$$
$$= \mathrm{Op}_\Sigma \{h, a\}_\Sigma + \tfrac{\varepsilon}{2} \mathrm{Op}_{\mathbb{R}^{2d}} \Big(\{ \mathrm{Op}_{\mathbb{S}^2} h_1, \mathrm{Op}_{\mathbb{S}^2} a \}_{\mathbb{R}^{2d}}$$
$$- \{ \mathrm{Op}_{\mathbb{S}^2} a, \mathrm{Op}_{\mathbb{S}^2} h_1 \}_{\mathbb{R}^{2d}} - 2\, \mathrm{Op}_{\mathbb{S}^2} \{h_1, a\}_{\mathbb{R}^{2d}} \Big) + \mathcal{O}(\varepsilon^2),$$

where the second term of order ε is a bounded operator and the remainder is order ε^2 as a bounded operator.

(ii)   Under the assumption of (ii), also the second term is of order ε^2, since

$$\begin{aligned}
&\left\{\mathrm{Op}_{\mathbb{S}^2}h_1, \mathrm{Op}_{\mathbb{S}^2}a\right\}_{\mathbb{R}^{2d}} - \left\{\mathrm{Op}_{\mathbb{S}^2}a, \mathrm{Op}_{\mathbb{S}^2}h_1\right\}_{\mathbb{R}^{2d}} - 2\,\mathrm{Op}_{\mathbb{S}^2}\{h_1, a\}_{\mathbb{R}^{2d}} \\
&= \left\{\mathrm{Op}_{\mathbb{S}^2}h_1, \mathrm{Op}_{\mathbb{S}^2}(a-a_0)\right\}_{\mathbb{R}^{2d}} - \left\{\mathrm{Op}_{\mathbb{S}^2}(a-a_0), \mathrm{Op}_{\mathbb{S}^2}h_1\right\}_{\mathbb{R}^{2d}} \\
&\quad - 2\,\mathrm{Op}_{\mathbb{S}^2}\{h_1, (a-a_0)\}_{\mathbb{R}^{2d}} \\
&= \mathcal{O}(\varepsilon).
\end{aligned}$$

(iii)   For the first equality in (iii), just note that there are no remainder terms in (2.15) and (2.16) in this case. In view of (2.10), $\mathrm{Op}_{\mathbb{S}^2}a = \mathrm{Op}_{\mathbb{S}^2}\mathcal{P}a$, we can replace a by $\mathcal{P}a$ in the above equation. Thus, both arguments of the Poisson brackets are linear in n and we conclude with the help of Lemma 2.5 that

$$\begin{aligned}
&\left\{\mathrm{Op}_{\mathbb{S}^2}h_1, \mathrm{Op}_{\mathbb{S}^2}a\right\}_{\mathbb{R}^{2d}} - \left\{\mathrm{Op}_{\mathbb{S}^2}a, \mathrm{Op}_{\mathbb{S}^2}h_1\right\}_{\mathbb{R}^{2d}} - 2\,\mathrm{Op}_{\mathbb{S}^2}\{h_1, a\}_{\mathbb{R}^{2d}} \\
&= R(h_1, a) - \mathrm{Op}_{\mathbb{S}^2}\{h_1, (1-\mathcal{P})a\}_{\mathbb{R}^{2d}} = -\mathrm{Op}_{\mathbb{S}^2}\{h_1, (1-\mathcal{P})a\}_{\mathbb{R}^{2d}}.
\end{aligned}$$

This proves the second equality in (iii).   □

All that remains is to prove the auxiliary Lemma 2.5:

Proof of Lemma 2.5. Let $a = \mathfrak{a}_0 + \sqrt{3}\,\mathfrak{a}\cdot n$ and $b = \mathfrak{b}_0 + \sqrt{3}\,\mathfrak{b}\cdot n$ be the scalar symbols to the matrix-valued functions $A = \mathfrak{a}_0\,\mathbf{1}_{\mathbb{C}^2} + \mathfrak{a}\cdot\sigma$ and $B = \mathfrak{b}_0\,\mathbf{1}_{\mathbb{C}^2} + \mathfrak{b}\cdot\sigma$. We can write the difference of the Poisson brackets as the difference of two anti-commutators,

$$\{A, B\}_{\mathbb{R}^d} - \{B, A\}_{\mathbb{R}^d} = \sum_{j=1}^{d}\left([\partial_{p_j}A, \partial_{q_j}B]_+ - [\partial_{p_j}A, \partial_{q_j}B]_+\right).$$

These anti-commutators can be expressed in terms of the coefficients,

$$\begin{aligned}
[A, B]_+ &= \left(\mathfrak{a}_0\,\mathbf{1}_{\mathbb{C}^2} + \mathfrak{a}\cdot\sigma\right)\left(\mathfrak{b}_0\,\mathbf{1}_{\mathbb{C}^2} + \mathfrak{b}\cdot\sigma\right) + \left(\mathfrak{b}_0\,\mathbf{1}_{\mathbb{C}^2} + \mathfrak{b}\cdot\sigma\right)\left(\mathfrak{a}_0\,\mathbf{1}_{\mathbb{C}^2} + \mathfrak{a}\cdot\sigma\right) \\
&= 2\left(\mathfrak{a}_0\,\mathfrak{b}_0 + \mathfrak{a}\cdot\mathfrak{b}\right)\mathbf{1}_{\mathbb{C}^2} + 2\left(\mathfrak{a}_0\,\mathfrak{b} + \mathfrak{b}_0\,\mathfrak{a}\right)\cdot\sigma.
\end{aligned}$$

By a straightforward computation, we can verify that $\mathcal{P}\big(3(\mathfrak{a}\cdot n)\,(\mathfrak{b}\cdot n)\big) = \mathfrak{a}\cdot\mathfrak{b}$ holds true and hence

$$\mathrm{Op}_{\mathbb{S}^2}\big(3(\mathfrak{a}\cdot n)\,(\mathfrak{b}\cdot n)\big) = \mathrm{Op}_{\mathbb{S}^2}\mathcal{P}\big(3(\mathfrak{a}\cdot n)\,(\mathfrak{b}\cdot n)\big) = (\mathfrak{a}\cdot\mathfrak{b})\,\mathbf{1}_{\mathbb{C}^2}.$$

This means the right-hand side of

$$\begin{aligned}
2\,\mathrm{Op}_{\mathbb{S}^2}\{a, b\}_{\mathbb{R}^d} &= 2\sum_{j=1}^{d}\mathrm{Op}_{\mathbb{S}^2}\left(\left(\partial_{p_j}\mathfrak{a}_0 + \sqrt{3}\,\partial_{p_j}\mathfrak{a}\cdot n\right)\left(\partial_{q_j}\mathfrak{b}_0 + \sqrt{3}\,\partial_{q_j}\mathfrak{b}\cdot n\right)\right) \\
&\quad + \text{other terms} \\
&= 2\sum_{j=1}^{d}\mathrm{Op}_{\mathbb{S}^2}\left(\left(\partial_{p_j}\mathfrak{a}_0\,\partial_{q_j}\mathfrak{b}_0 + 3\left(\partial_{p_j}\mathfrak{a}\cdot n\right)\left(\partial_{q_j}\mathfrak{b}\cdot n\right)\right)\right)
\end{aligned}$$

$$+ \sqrt{3} \left(\partial_{q_j} \mathfrak{b}_0 \, \partial_{p_j} \mathfrak{a} + \partial_{p_j} \mathfrak{a}_0 \, \mathfrak{b} \right) \cdot n \Big) + \text{other terms}$$

$$= \sum_{j=1}^{d} \left([\partial_{p_j} A , \partial_{q_j} B]_+ - [\partial_{q_j} A , \partial_{p_j} B]_+ \right)$$

agrees with $\{A, B\}_{\mathbb{R}^d} - \{B, A\}_{\mathbb{R}^d}$, and $R(a, b)$ vanishes identically. $\square$

3. Egorov Theorems

Suppose h satisfies Assumption 2.3 and denotes by Φ^ε the Hamiltonian flow associated to Hamilton's equation of motion

$$\dot{q} = +\nabla_p h = +\nabla_p h_0 + \varepsilon \left(\nabla_p \mathfrak{h}_0 + \sqrt{3} \, \nabla_p (\mathfrak{h} \cdot n) \right)$$

$$\dot{p} = -\nabla_q h = -\nabla_q h_0 - \varepsilon \left(\nabla_q \mathfrak{h}_0 + \sqrt{3} \, \nabla_q (\mathfrak{h} \cdot n) \right) \qquad (3.1)$$

$$\dot{n} = 2\,\mathfrak{h} \wedge n$$

on extended phase space $\Sigma = \mathbb{R}^{2d} \times \mathbb{S}^2$. To shorten the notation, we will often use $z = (q, p) \in \mathbb{R}^{2d}$ for the translational variables and ∂_z stands for either ∂_{q_j} or ∂_{p_j}. Then, the Hamiltonian flow $\Phi_t^\varepsilon = \left(Z^\varepsilon(t), N^\varepsilon(t) \right)$ similarly splits into a translational part $Z^\varepsilon(t) = \left(Q^\varepsilon(t), P^\varepsilon(t) \right)$ and spin $N^\varepsilon(t)$. It is easy to see that under the assumptions placed on h, the flow Φ^ε exists globally in time and is smooth (Proposition 4.1).

If we replace h by the leading-order term h_0 in the first two equations of (3.1), we obtain the *skew product flow* Φ^0 from [2]; this flow also exists for all $t \in \mathbb{R}$, is smooth and agrees with the *Hamiltonian* flow $\Phi_t^\varepsilon = \Phi_t^0 + \mathcal{O}(\varepsilon)$ to leading order for all bounded times. We will write $\Phi_t^0 = \left(Z^0(t), N^0(t) \right)$ for the translational and spin part. Here, translational and spin dynamics decouple and there is no back-reaction from the spin dynamics onto the translational dynamics, the spin is just "dragged along".

Now, we have the necessary terminology to prove our semiclassical limits: combining standard Weyl and Stratonovich–Weyl calculus with standard arguments, we obtain an Egorov theorem for times of order 1. The proofs of the relevant properties of the flow are postponed to Sect. 4.

Theorem 3.1 ($\mathcal{O}(1)$-time Egorov-type theorem). *Suppose h satisfies $\mathfrak{h}_0 \in S^0$ in addition to Assumption 2.3. Then, for any $a \in S_\Sigma^0$ and $T < \infty$, the following two statements hold:*

(i) $\quad \displaystyle\sup_{t \in [-T,T]} \left\| \mathrm{e}^{+\mathrm{i}\hat{h}\frac{t}{\varepsilon}} \, \mathrm{Op}_\Sigma(a) \, \mathrm{e}^{-\mathrm{i}\hat{h}\frac{t}{\varepsilon}} - \mathrm{Op}_\Sigma\left(a \circ \Phi_t^\varepsilon \right) \right\|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}(\varepsilon)$

(ii) *If in addition a is independent of n, then the error is of second order,*

$$\sup_{t \in [-T,T]} \left\| \mathrm{e}^{+\mathrm{i}\hat{h}\frac{t}{\varepsilon}} \, \mathrm{Op}_\Sigma(a) \, \mathrm{e}^{-\mathrm{i}\hat{h}\frac{t}{\varepsilon}} - \mathrm{Op}_\Sigma\left(a \circ \Phi_t^\varepsilon \right) \right\|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}(\varepsilon^2).$$

Proof. (i) By Proposition 4.1, the flow Φ^ε exists and all its derivatives are bounded for all $|t| \leq T$. We abbreviate the classically evolved observable with $a(t) := a \circ \Phi_t^\varepsilon$ and set $\hat{a} := \mathrm{Op}_\Sigma(a)$. Then, a Duhamel argument yields

$$\mathrm{e}^{\mathrm{i}\hat{h}\frac{t}{\varepsilon}}\,\hat{a}\,\mathrm{e}^{-\mathrm{i}\hat{h}\frac{t}{\varepsilon}} \;-\; \widehat{a(t)} = \int_0^t \mathrm{d}s\, \frac{\mathrm{d}}{\mathrm{d}s}\left(\mathrm{e}^{\mathrm{i}\frac{s}{\varepsilon}\hat{h}}\,\widehat{a(t-s)}\,\mathrm{e}^{-\mathrm{i}\frac{s}{\varepsilon}\hat{h}}\right)$$

$$= \int_0^t \mathrm{d}s\,\mathrm{e}^{\mathrm{i}\frac{s}{\varepsilon}\hat{h}}\left(\tfrac{\mathrm{i}}{\varepsilon}\big[\hat{h},\widehat{a(t-s)}\big] + \tfrac{\mathrm{d}}{\mathrm{d}s}\,\widehat{a(t-s)}\right)\mathrm{e}^{-\mathrm{i}\frac{s}{\varepsilon}\hat{h}}$$

$$= \int_0^t \mathrm{d}s\,\mathrm{e}^{\mathrm{i}\frac{s}{\varepsilon}\hat{h}}\left(\tfrac{\mathrm{i}}{\varepsilon}\big[\hat{h},\widehat{a(t-s)}\big] - \mathrm{Op}_\Sigma\{h,a(t-s)\}_\Sigma\right)\mathrm{e}^{-\mathrm{i}\frac{s}{\varepsilon}\hat{h}}. \qquad (3.2)$$

Combining Corollary 4.2 with the usual Caldéron–Vaillancourt theorem [18, Théorème II 36] and Lemma 2.4 (i), we obtain

$$\sup_{t\in[-T,T]}\left\|\tfrac{\mathrm{i}}{\varepsilon}\big[\hat{h},\widehat{a(t-s)}\big] - \mathrm{Op}_\Sigma\{h,a(t-s)\}_\Sigma\right\|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}(\varepsilon)$$

and thus we have shown (i).

(ii)   If $a(q,p,n) = a(q,p)$, then $a_1(t) := a\circ\Phi_t^\varepsilon - a\circ\Phi_t^0 = \mathcal{O}(\varepsilon)$ by Proposition 4.1 where Φ^0 is the decoupled flow introduced in the beginning of the section. Thus Lemma 2.4 (ii) applies and

$$\sup_{t\in[-T,T]}\left\|\tfrac{\mathrm{i}}{\varepsilon}\big[\hat{h},\widehat{a(t-s)}\big] - \mathrm{Op}_\Sigma\{h,a(t-s)\}_\Sigma\right\|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}(\varepsilon^2)$$

holds which in turn implies (ii).   □

Note that (i) just shows that we can replace the skew product flow (1.3) with the Hamiltonian flow Φ^ε without changing the size of the error. For purely translational observables, one can improve the error estimate by a factor of ε when going from the skew product flow to Φ^ε.

As an immediate corollary, we obtain a semiclassical limit for states: here we compare $\hat{\rho}(t) = \mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}\hat{h}}\,\hat{\rho}\,\mathrm{e}^{+\mathrm{i}\frac{t}{\varepsilon}\hat{h}}$ with $\mathcal{W}_\Sigma(\hat{\rho})\circ\Phi_{-t}^\varepsilon$, where $\mathcal{W}_\Sigma(\hat{\rho})$ is the Wigner transform of the density operator $\hat{\rho}$.

Corollary 3.2. *In addition to the conditions of Theorem 3.1, assume that $\hat{\rho}$ is a density operator with Wigner transform $W := \mathcal{W}_\Sigma(\hat{\rho})$.*

(i)   *If $a \in S_\Sigma^0$ depends non-trivially on spin, then*

$$\mathrm{Tr}\big(\mathrm{Op}_\Sigma(a)\,\hat{\rho}(t)\big) = \frac{1}{(2\pi)^d}\,\frac{1}{4\pi}\int_{\mathbb{R}^{2d}}\mathrm{d}q\,\mathrm{d}p\int_{\mathbb{S}^2}\mathrm{d}n\,a(q,p,n)\,W\circ\Phi_{-t}^\varepsilon(q,p,n)$$
$$+ \mathcal{O}(\varepsilon)$$

holds for all $|t| \le T$.

(ii)   *If $a \in S_\Sigma^0$ is independent of n, then*

$$\mathrm{Tr}\big(\mathrm{Op}_\Sigma(a)\,\hat{\rho}(t)\big) = \frac{1}{(2\pi)^d}\,\frac{1}{4\pi}\int_{\mathbb{R}^{2d}}\mathrm{d}q\,\mathrm{d}p\int_{\mathbb{S}^2}\mathrm{d}n\,a(q,p,n)\,W\circ\Phi_{-t}^\varepsilon(q,p,n)$$
$$+ \mathcal{O}(\varepsilon^2)$$

holds for all $|t| \le T$.

Proof. The proofs of (i) and (ii) rely on Theorem 3.1,

$$\mathrm{Tr}\big(\mathrm{Op}_\Sigma(a)\,\hat\rho(t)\big) = \mathrm{Tr}\left(\mathrm{Op}_\Sigma(a)\,\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}\hat h}\,\hat\rho\,\mathrm{e}^{+\mathrm{i}\frac{t}{\varepsilon}\hat h}\right) = \mathrm{Tr}\left(\mathrm{e}^{+\mathrm{i}\frac{t}{\varepsilon}\hat h}\,\mathrm{Op}_\Sigma(a)\,\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}\hat h}\,\hat\rho\right),$$

the observation that $\hat\rho(t)$ and $W\circ\Phi_t^\varepsilon$ solve the equations of motion for observables backwards in time and Liouville's theorem. $\qquad\square$

Attempting to extend Egorov theorems to longer time scales is hard and requires more detailed information on the flow. The non-linearity of the classical system limits the time scale of validity of semiclassical approximations to the Ehrenfest time $t = \mathcal{O}(|\ln\varepsilon|)$. While for quadratic Hamiltonians on phase-space $\mathbb{R}^{2d}$, one finds that $\hat A(t) = \mathrm{Op}\big(A\circ\Phi_t^0\big)$ holds without error since the equations of motion are *linear*, any coupling between translational and spin degrees of freedom introduces additional non-linear terms for the equations of motion on *extended* phase space. However, in the case that h_0 is a quadratic polynomial in the components of p and q, and the components of $\mathfrak{h}_0$ and $\mathfrak{h}$ are linear polynomials in q and p, we can still find bounds on the derivatives of the flow for times of order $\mathcal{O}(\varepsilon^{-\gamma})$ for some $\gamma > 0$ (cf. Proposition 4.3). The Jaynes–Cummings- and Rabi-type Hamiltonians which, among other things, describe the interaction between an electromagnetic mode in a cavity and an atomic two-level system, are of this type.

A second important ingredient in our long-time semiclassical limit involves using suitable boundedness criteria for ΨDOs: the usual Caldéron–Vaillancourt theorem [18, Théorème II 36] requires us to control $2d + 1$ derivatives where d is the dimension of translational configuration space, i.e. there exists a constant $c_d > 0$ depending only on d such that

$$\big\|\mathrm{Op}_\Sigma(a)\big\|_{\mathcal{B}(\mathcal{H})} \le c_d\,\|a\|_{0,2d+1}$$

holds for all $a \in S_\Sigma^0$ uniformly in $\varepsilon \in (0,\varepsilon_0)$. To reduce the number of derivatives, we will use other bounds: if a decays sufficiently rapidly at ∞, we only need to control $d + 1$ derivatives. More specifically, a straightforward generalization of [10, Lemma 1.1] and [8, Lemma 3.1] to matrix-valued symbols gives the following estimate:

$$\big\|\mathrm{Op}_\Sigma(a)\big\|_{\mathcal{B}(\mathcal{H})} \le c_d \max_{|\alpha|\le d+1} \sup_{(q,p,n)\in\Sigma}\left(\langle p\rangle^{d+1}\,\big|\partial_p^\alpha a(q,p,n)\big|\right). \qquad (3.3)$$

Again, the constant $c_d > 0$ depends only on d and is uniform in $\varepsilon \in (0,\varepsilon_0)$. Finally, for compactly supported symbols $a \in \mathcal{C}_\mathrm{c}^\infty(\Sigma)$, we can give a bound which only involves the sup norm,

$$\big\|\mathrm{Op}_\Sigma(a)\big\|_{\mathcal{B}(\mathcal{H})} \le \frac{c_d}{\varepsilon^{d/2}}\,\mathrm{Vol}\big(\mathrm{supp}\,a\big) \sup_{(q,p,n)\in\Sigma} |a(q,p,n)|. \qquad (3.4)$$

It is the last two boundedness criteria which enter the proof of the long-time semiclassical limit.

Theorem 3.3 (Long-time Egorov theorem). *Let $d = 1$, $h_0(q,p) = \frac{1}{2}\big(p^2 + \omega^2 q^2\big)$, $\mathfrak{h}_0 = 0$ and $\mathfrak{h}$ be a linear polynomial in q and p. Then, for any $T < \infty$, the following statements hold:*

(i) *Suppose $a \in S_\Sigma^{-2}$. Then, for any $\gamma < 1/4$, there is $\varepsilon_0 > 0$ such that for $\varepsilon < \varepsilon_0$*

$$\sup_{|t| \in [0, T/\varepsilon^\gamma]} \left\| e^{+i\frac{t}{\varepsilon}\hat{h}} \operatorname{Op}_\Sigma(a) e^{-i\frac{t}{\varepsilon}\hat{h}} - \operatorname{Op}_\Sigma(a \circ \Phi_t^\varepsilon) \right\|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}(\varepsilon^{1-4\gamma}). \quad (3.5)$$

(ii) *If in addition $a \in \mathcal{C}_c^\infty(\Sigma)$ is independent of n, then for any $\gamma < 1/2$ there is $\varepsilon_0 > 0$ such that for $\varepsilon < \varepsilon_0$ we have*

$$\sup_{|t| \in [0, T/\varepsilon^\gamma]} \left\| e^{+i\frac{t}{\varepsilon}\hat{h}} \operatorname{Op}_\Sigma(a) e^{-i\frac{t}{\varepsilon}\hat{h}} - \operatorname{Op}_\Sigma(a \circ \Phi_t^\varepsilon) \right\|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}(\varepsilon^{3/2-3\gamma}). \quad (3.6)$$

Proof. (i) Assume $t = \mathcal{O}(\varepsilon^{-\gamma})$ for some $\gamma \geq 0$ that has yet to be determined. Moreover, let $b, g > 0$ be the constants defined in the proof of Proposition 4.3 and $\alpha = 1/2$. Lastly, for better readability, define the remainder

$$R(a(t)) := -\operatorname{Op}_{\mathbb{S}^2}\{h_1, (1-\mathcal{P})a(t)\}_{\mathbb{R}^{2d}}$$

which involves first-order derivatives of $a(t)$ in q and p. Then, the chain rule

$$\partial_z(a \circ \Phi_t^\varepsilon)(z,n) = Da(\Phi_t^\varepsilon(z,n)) \partial_z \Phi_t^\varepsilon(z,n)$$

and analogous expressions for higher order derivatives, equation (3.2), Lemma 2.4 (iii) and boundedness criterion (3.3) imply

$$\sup_{|t| \in [0, T/\varepsilon^\gamma]} \left\| e^{+i\frac{t}{\varepsilon}\hat{h}} \operatorname{Op}_\Sigma(a) e^{-i\frac{t}{\varepsilon}\hat{h}} - \operatorname{Op}_\Sigma(a \circ \Phi_t^\varepsilon) \right\|_{\mathcal{B}(\mathcal{H})}$$

$$\leq \varepsilon \int_0^t ds \left\| \operatorname{Op}_{\mathbb{R}^{2d}}(R(a(t))) \right\|_{\mathcal{B}(\mathcal{H})}$$

$$\leq \varepsilon |t| C \max_{|\alpha| \leq 3} \sup_{(z,n) \in \Sigma} \left(\langle p \rangle^2 \left\| \partial_z^\alpha (a \circ \Phi_t^\varepsilon)(z,n) \right\| \right).$$

Proposition 4.3 allows us to estimate the right-hand side by

$$\max_{|\alpha| \leq 3} \sup_{(z,n) \in \Sigma} \left(\langle p \rangle^2 \left\| \partial_z^\alpha (a \circ \Phi_t^\varepsilon)(z,n) \right\| \right) \leq C \left(1 + |t|^3 \right)$$

for $|t| \leq \varepsilon^{-1/2} \sqrt{2bg}^{-1}$. Hence, for $t = \mathcal{O}(\varepsilon^{-\gamma})$, $\gamma < 1/4$, we obtain the bound

$$\sup_{|t| \in [0, T/\varepsilon^\gamma]} \left\| e^{+i\frac{t}{\varepsilon}\hat{h}} \operatorname{Op}_\Sigma(a) e^{-i\frac{t}{\varepsilon}\hat{h}} - \operatorname{Op}_\Sigma(a \circ \Phi_t^\varepsilon) \right\|_{\mathcal{B}(\mathcal{H})}$$

$$\leq \varepsilon C \left(|t| + |t|^4 \right) = \mathcal{O}(\varepsilon^{1-4\gamma}).$$

(ii) Again let $t = \mathcal{O}(\varepsilon^{-\gamma})$ for some $\gamma \geq 0$ that has yet to be determined. In case a is initially independent of n and has compact support, we have $a(t,z,n) = a(Z^\varepsilon(t,z,n))$ and thus

$$\partial_z a(t,z,n) = Da(Z^\varepsilon(t,z,n)) \partial_z Z^\varepsilon(t,z,n).$$

Since the volume measure on phase space coincides with the Liouville measure, the above equation combined with Liouville's Theorem implies that for all $t \in \mathbb{R}$, we have

$$\mathrm{Vol}\big(\mathrm{supp}\, \partial_z a(t)\big) \leq \mathrm{Vol}\big(\mathrm{supp}\, a(t)\big) = \mathrm{Vol}\big(\mathrm{supp}\, a\big).$$

The function $a_0(t) := a \circ \Phi_t^0$ is independent of n and thus $\mathcal{P}a_0(t) = a_0(t)$ holds for all t. This means, we can insert $a_0(t)$ into the remainder and estimate its norm for times $|t| \leq \varepsilon^{-1/2}\sqrt{2bg}^{-1}$ using equation (3.4) and Proposition 4.3,

$$\varepsilon\, |t| \sup_{|s|\in[0,t]} \left\| \mathrm{Op}_{\mathbb{R}^{2d}}\Big(R\big(a(t) - a_0(t)\big)\Big)\right\|_{\mathcal{B}(\mathcal{H})}$$

$$\leq \varepsilon\, |t|\, \frac{C}{\sqrt{\varepsilon}} \max_{|\alpha|\leq 1} \sup_{|s|\in[0,t]} \sup_{(z,n)\in\Sigma}$$

$$\Big(\big|Da\big(Z^\varepsilon(s,z,n)\big) - Da\big(Z^0(s,z)\big)\big|\, \big|\partial_z^\alpha Z(s,z,n)\big|$$

$$+ \big|Da\big(Z^0(s,z)\big)\big|\, \big|\partial_z^\alpha\big(Z^\varepsilon(s,z,n) - Z^0(s,z)\big)\big|\Big)$$

$$\leq \sqrt{\varepsilon}\, C\, |t|\, \big(\varepsilon\, |t| + \varepsilon\, bg\, |t|^3\big) = \mathcal{O}\big(\varepsilon^{3/2 - 3\gamma}\big).$$

Hence, as long as $t = \mathcal{O}(\varepsilon^{-\gamma})$ for $\gamma < 1/2$, the right-hand side goes to 0 as $\varepsilon \to 0$ and we have shown (ii). $\square$

In the special case of a quadratic Hamiltonian, we can actually get an exact equation for the time-evolution of the symbol of a semiclassical operator, albeit not in terms of a classical flow.

Theorem 3.4. *Let $d = 1$ and $h_0(q,p) = \frac{1}{2}\big(p^2 + \omega^2 q^2\big)$, $\mathfrak{h}_0 = 0$ and $\mathfrak{h}$ be a polynomial in q and p of degree 1. Let $a \in S_\Sigma^{-2}$ and $a(t,q,p,n)$ be a solution of*

$$\partial_t a(t,q,p,n) = \big(\mathcal{P}\{h,a(t)\}_\Sigma\big)(q,p,n)$$

such that $a(t) \in S_\Sigma^0$ for all $t \in \mathbb{R}$. Then,

$$\mathrm{e}^{\mathrm{i}\hat{h}\frac{t}{\varepsilon}}\, \hat{a}\, \mathrm{e}^{-\mathrm{i}\hat{h}\frac{t}{\varepsilon}} = \mathrm{Op}_\Sigma\big(a(t)\big). \tag{3.7}$$

Proof. By definition $a(t,q,p,\cdot) \in C_1(\mathbb{S}^2)$ for all $t \in \mathbb{R}$. Thus, by Lemma 2.4 (iii) we have

$$\tfrac{\mathrm{i}}{\varepsilon}\big[\mathrm{Op}_\Sigma h, \mathrm{Op}_\Sigma a(t)\big] = \mathrm{Op}_\Sigma\{h,a(t)\}_\Sigma = \mathrm{Op}_\Sigma \mathcal{P}\{h,a(t)\}_\Sigma = \mathrm{Op}_\Sigma\big(\dot{a}(t)\big).$$

                                                    $\square$

4. Estimates on the Classical Flow

In this section, we study properties of the flows Φ^ε and Φ^0 as defined in the beginning of Sect. 3: $\Phi_t^\varepsilon = \big(Z^\varepsilon(t), N^\varepsilon(t)\big)$ is the Hamiltonian flow associated to (3.1) while $\Phi_t^0 = \big(Z^0(t), N^0(t)\big)$ is the flow associated to (3.1) after replacing h by h_0 in the first two equations. Existence for all times and smoothness follows from standard arguments from the theory of ordinary differential equations.

Proposition 4.1. *Suppose h satisfies* $\mathfrak{h} \in S^0$ *in addition to Assumption 2.3. Then,* Φ^ε *and* Φ^0 *exist globally in time and are smooth, i.e. for any* $t \in \mathbb{R}$, Φ^ε *and* Φ^0 *are diffeomorphisms on* Σ *and depend smoothly on time. Moreover, for bounded time intervals* $[-T, +T]$*, we have* $\Phi_t^\varepsilon = \Phi_t^0 + \mathcal{O}(\varepsilon)$ *and all partial derivatives* $\partial_z^\alpha \partial_n^\beta \Phi_t^\varepsilon$ *and* $\partial_z^\alpha \partial_n^\beta \Phi_t^0$ *are uniformly bounded.*

Proof. All claims follow from the fact that the vector fields (r.h.s. of (3.1)) have globally bounded derivatives to all orders. Moreover, the difference between the vector fields which define Φ^ε and Φ^0 is bounded and $\mathcal{O}(\varepsilon)$, and thus the Grönwall lemma implies $\Phi_t^\varepsilon = \Phi_t^0 + \mathcal{O}(\varepsilon)$ for bounded time intervals. $\qquad\square$

This immediately implies that the actions of Φ^ε and Φ^0 preserve Hörmander classes.

Corollary 4.2. *Let h satisfies Assumption 2.3 and, in addition, let* $\mathfrak{h} \in S^0$. *Then, for* $a \in S_\Sigma^k(\varepsilon)$ *it holds that* $a \circ \Phi_t^\varepsilon, a \circ \Phi_t^0 \in S_\Sigma^k(\varepsilon)$ *for all* $t \in \mathbb{R}$ *and for any* $T < \infty$ *and* $r \in \mathbb{N}_0$

$$\sup_{t \in [-T,T]} \sup_{\varepsilon \in (0,\varepsilon_0)} \left\| a \circ \Phi_t^\varepsilon \right\|_{k,r} < \infty \qquad and \qquad \sup_{t \in [-T,T]} \sup_{\varepsilon \in (0,\varepsilon_0)} \left\| a \circ \Phi_t^0 \right\|_{k,r} < \infty.$$

Now, let us turn to the case of Jaynes–Cummings- and Rabi-type Hamiltonians. If $\mathfrak{h}$ is the prefactor of $h_1 = \sqrt{3}\,\mathfrak{h} \cdot n$, we define the skew symmetric matrix

$$\mathfrak{H} := 2 \begin{pmatrix} 0 & -\mathfrak{h}_3 & +\mathfrak{h}_2 \\ +\mathfrak{h}_3 & 0 & -\mathfrak{h}_1 \\ -\mathfrak{h}_2 & +\mathfrak{h}_1 & 0 \end{pmatrix}.$$

This convention allows us to write down proofs of the long-time flow estimates in a more compact fashion.

Proposition 4.3. *Let* $d = 1$ *and*

$$h_0(q,p) = \tfrac{1}{2}\left(p^2 + \omega^2 q^2\right), \qquad h_1(q,p,n) = \sqrt{3}\left(\mathfrak{h}_c + q\,\mathfrak{h}_q + p\,\mathfrak{h}_p\right) \cdot n,$$

where $\mathfrak{h}_c, \mathfrak{h}_q, \mathfrak{h}_p \in \mathbb{R}^3$. *Then, the flows* Φ^ε *and* Φ^0 *exist globally in time and the two are* $\mathcal{O}(\varepsilon)$*-close,*

$$\sup_{(z,n) \in \Sigma} \left| Z^\varepsilon(t,z,n) - Z^0(t,z) \right| = \mathcal{O}\left(\varepsilon\,|t|\right),$$

$$\sup_{(z,n) \in \Sigma} \left| N^\varepsilon(t,z,n) - N^0(t,z,n) \right| = \mathcal{O}\left(\varepsilon\,|t|^2\right).$$

We abbreviate $Z = Z^\varepsilon$ *and* $N = N^\varepsilon$ *and introduce the norms*

$$\|X\|_t := \sup_{s \in [-t,t]} \left| X(s) \right|.$$

Let $'$ *denote a derivative with respect to either q or p. Then, there are constants* $b, g > 0$ *depending only on* h_1 *such that for any* $0 < \alpha < 1$ *and all* $|t| \leq \varepsilon^{-1/2}\sqrt{\frac{\alpha}{bg}}$ *it holds that*

$$\left\|Z'\right\|_t \leq \frac{1}{1-\alpha}, \qquad\qquad \left\|N'\right\|_t \leq \frac{b|t|}{1-\alpha},$$

$$\left\|Z''\right\|_t \leq \frac{\alpha b|t|}{(1-\alpha)^3}, \qquad\qquad \left\|N''\right\|_t \leq \frac{b^2|t|^2}{(1-\alpha)^3},$$

$$\left\|Z'''\right\|_t \leq \frac{4\alpha b^2|t|^2}{(1-\alpha)^5}, \qquad\qquad \left\|N'''\right\|_t \leq \frac{4b^3|t|^3}{(1-\alpha)^5},$$

and

$$\left\|Z' - Z^{0'}\right\|_t \leq \frac{\varepsilon\, bg|t|^2}{1-\alpha}.$$

Proof. To write the equations of motion in a concise form, we abbreviate

$$\Omega = \begin{pmatrix} 0 & 1 \\ -\omega^2 & 0 \end{pmatrix} \quad \text{and} \quad G = \sqrt{3}\begin{pmatrix} +\mathfrak{h}_p^T \\ -\mathfrak{h}_q^T \end{pmatrix}.$$

Then,

$$\dot{Z} = \Omega Z + \varepsilon GN\,, \qquad \dot{N} = \mathfrak{H}(Z)N = \mathfrak{H}(Z^0)N + \mathfrak{H}(Z - Z^0)N. \qquad (4.1)$$

Let $R_Z(t) \in SO(2)$ be the propagator of the harmonic oscillator satisfying $\dot{R}_Z(t) = \Omega R_Z(t)$ with $R_Z(0) = \mathbf{1}_{\mathbb{R}^2}$, then the "variation of constants" formula gives

$$Z(t) = R_Z(t)\left(Z(0) + \varepsilon\int_0^t \mathrm{d}s\, R_Z(-s)\, G\, N(s) \right)$$

$$= Z^0(t) + \varepsilon\int_0^t \mathrm{d}s\, R_Z(t-s)\, G\, N(s).$$

Thus, $\sup_{(q,p,n)\in\Sigma}\left|Z(t,q,p,n) - Z^0(t,q,p)\right| = \mathcal{O}(\varepsilon|t|)$. For N, we find analogously with $A_0(t) \in SO(3)$ the propagator of the "homogeneous" system

$$\dot{A}_0(t) = \mathfrak{H}(Z^0(t))A_0(t)$$

that

$$N(t) = A_0(t)\left(N(0) + \int_0^t \mathrm{d}s\, A_0(-s)\, \mathfrak{H}(Z(s) - Z^0(s))\, N(s) \right)$$

$$= N^0(t) + \int_0^t \mathrm{d}s\, A_0(t-s)\, \mathfrak{H}(Z(s) - Z^0(s))\, N(s)$$

and thus $\sup_{(q,p,n)\in\Sigma}\left|N(t,q,p,n) - N^0(t,q,p,n)\right| = \mathcal{O}(\varepsilon|t|^2)$.

We now turn to the derivatives of the flow. Let $'$ be a derivative with respect to the initial q or p. Then, the derivatives of the flow map satisfy the equations

$$\dot{Z}' = \Omega Z' + \varepsilon G N', \qquad \dot{N}' = \mathfrak{H}(Z)N' + B(Z')N,$$

where $B(Z')$ is a skew-symmetric matrix with all components linear in Q' and P'. Let $R_Z(t) \in SO(2)$ be as before and $R_N(t) \in SO(3)$ be the propagator of the "homogeneous" system

$$\dot{R}_N(t) = \mathfrak{H}(Z(t))R_N(t),$$

then the variation of constants formula and $\Phi_0^\varepsilon(z, n) = (z, n)$ gives

$$Z'(t) = R_Z(t)\left(Z'(0) + \varepsilon \int_0^t ds\, R_Z(-s)\, G\, N'(s)\right)$$

$$N'(t) = R_N(t)\Big(\underbrace{N'(0)}_{=0} + \int_0^t ds\, R_N(-s)\, B(Z'(s))\, N(s)\Big)$$

$$= \int_0^t ds\, R_N(t-s)\, B(Z'(s))\, N(s).$$

From this, we infer that

$$\left\| Z'\right\|_t \le \underbrace{\left| Z'(0)\right|}_{=1} + \varepsilon\, g|t|\,\left\| N'\right\|_t = 1 + \varepsilon\, g|t|\,\left\| N'\right\|_t$$

$$\left\| N'\right\|_t \le b|t|\,\left\| Z'\right\|_t$$

where $g = \|G\|_{\mathcal{B}(\mathbb{R}^3, \mathbb{R}^2)}$ and b is a constant depending on B. Combining these estimates, we find that for any $\alpha < 1$

$$\left\| Z'\right\|_t \le \frac{1}{1 - \varepsilon\, bg|t|^2} \le \frac{1}{1 - \alpha} \quad \text{and} \quad \left\| N'\right\|_t \le \frac{b|t|}{1 - \varepsilon\, bg|t|^2} \le \frac{b|t|}{1 - \alpha}$$

uniformly for $|t| \le \sqrt{\frac{\alpha}{\varepsilon g b}}$. Similarly, from

$$\dot{Z}' - \dot{Z}^{0'} = \varepsilon G N',$$

and the norm estimate for N', we deduce

$$\left\| Z' - Z^{0'}\right\|_t \le \varepsilon\, g\, |t|\, \|N'\|_t \le \frac{\varepsilon\, bg\, |t|^2}{1 - \alpha}.$$

Bounds on higher derivatives are obtained in the same way:

$$\dot{Z}'' = \Omega Z'' + \varepsilon G N''$$

$$\dot{N}'' = \mathfrak{H}(Z)N'' + B(Z'')N + B(Z')N'$$

implies

$$\left\| Z''\right\|_t \le \left| Z''(0)\right| + \varepsilon\, g|t|\,\left\| N''\right\|_t = \varepsilon\, g|t|\,\left\| N''\right\|_t$$

$$\left\| N''\right\|_t \le b|t|\left(\left\| Z''\right\|_t + \left\| Z'\right\|_t \left\| N'\right\|_t\right) \le b|t|\left(\left\| Z''\right\|_t + \frac{b\,|t|}{(1 - \alpha)^2}\right)$$

and thus

$$\left\|N''\right\|_t \le \varepsilon \, bg|t|^2 \left\|N''\right\|_t + \frac{b^2 \, |t|^2}{(1-\alpha)^2}.$$

Solving for $\left\|N''\right\|_t$ gives

$$\left\|N''\right\|_t \le \frac{1}{1-\varepsilon \, bg|t|^2} \, \frac{b^2|t|^2}{(1-\alpha)^2} \le \frac{b^2|t|^2}{(1-\alpha)^3}$$

and

$$\left\|Z''\right\|_t \le \frac{\varepsilon \, b^2 g|t|^3}{(1-\alpha)^3} \le \frac{\alpha b|t|}{(1-\alpha)^3}.$$

For the third derivatives, we find

$$\dot{Z}''' = \Omega Z''' + \varepsilon G N'''$$
$$\dot{N}''' = \mathfrak{H}(Z)N''' + B(Z''')N + 2B(Z')N'' + 2B(Z'')N'$$

and thus

$$\left\|Z'''\right\|_t \le \varepsilon \, g|t| \left\|N'''\right\|_t$$
$$\left\|N'''\right\|_t \le b|t| \left(\left\|Z'''\right\|_t + 2 \left\|Z'\right\|_t \left\|N''\right\|_t + 2 \left\|Z''\right\|_t \left\|N'\right\|_t \right)$$
$$\le b|t| \left(\left\|Z'''\right\|_t + \frac{2b^2|t|^2}{(1-\alpha)^4} + \frac{2\varepsilon \, b^3 g|t|^4}{(1-\alpha)^4} \right)$$
$$\le \varepsilon \, bg|t|^2 \left\|N'''\right\|_t + \frac{2b^3|t|^3 \, (1+\varepsilon \, bg|t|^2)}{(1-\alpha)^4}$$
$$\le \varepsilon \, bg|t|^2 \left\|N'''\right\|_t + \frac{4b^3|t|^3}{(1-\alpha)^4}$$

where in the last step we have used $0 < \alpha < 1$ and $|t| \le \varepsilon^{-1/2} \sqrt{\frac{\alpha}{bg}}$. Solving again for N''', we find

$$\left\|N'''\right\|_t \le \frac{4b^3|t|^3}{(1-\alpha)^5} \quad \text{and} \quad \left\|Z'''\right\|_t \le \frac{4\varepsilon \, b^3 g|t|^4}{(1-\alpha)^5} \le \frac{4\alpha b^2|t|^2}{(1-\alpha)^5}.$$

$\square$

5. The Stern–Gerlach Experiment

To illustrate our method, we discuss how the Stern–Gerlach experiment can be understood in terms of the semiclassical flow on extended phase space $\Sigma = \mathbb{R}^6 \times \mathbb{S}^2$. In this famous experiment, neutral atoms with magnetic moment g and spin-$1/2$ are sent through a weak, inhomogeneous magnetic field $\mathbf{B} = (\mathbf{B}_1, \mathbf{B}_2, \mathbf{B}_3) \in \mathcal{C}_b^\infty(\mathbb{R}^3, \mathbb{R}^3)$. For simplicity, we will absorb g into $\mathbf{B}$. In the experiment one observes that a beam of such particles splits into two parts

with intensities depending on the initial spin-state. The Hamiltonian describing a single atom in the beam is the Weyl quantization of

$$H(q,p) = \tfrac{1}{2}p^2 - \varepsilon\,\tfrac{1}{2}\mathbf{B}(q)\cdot\sigma$$
$$= \mathrm{Op}_{\mathbb{S}^2}\Big(\tfrac{1}{2}p^2 - \varepsilon\,\tfrac{\sqrt{3}}{2}\mathbf{B}(q)\cdot n\Big) =: \mathrm{Op}_{\mathbb{S}^2}\big(h(q,p,\cdot)\big). \qquad (5.1)$$

Due to the assumption on the magnetic field and the fact that the leading-order term of $H(q,p)$ is quadratic, Theorem 3.1 applies and for observables $a \in S^0_\Sigma$ which are initially independent of spin, we have a semiclassical limit with error $\mathcal{O}(\varepsilon^2)$. In particular, this implies that we can compute quantum expectation values

$$\mathrm{Tr}_{L^2(\mathbb{R}^3,\mathbb{C}^2)}\Big(\mathrm{e}^{+\mathrm{i}\frac{t}{\varepsilon}\hat{h}}\,\mathrm{Op}_\Sigma(a)\,\mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon}\hat{h}}\,\hat{w}\Big)$$
$$= \frac{1}{(2\pi)^3}\int_{\mathbb{R}^6}\mathrm{d}q\,\mathrm{d}p\,\frac{1}{4\pi}\int_{\mathbb{S}^2}\mathrm{d}n\,a\circ\Phi^\varepsilon_t(q,p,n)\,w(q,p,n) + \mathcal{O}(\varepsilon^2)$$

with respect to the state $\hat{w} = \mathrm{Op}_\Sigma(w)$ for times of order 1.

To be able to solve the semiclassical equations of motion (3.1) analytically, we will make some simplifying assumptions: first of all, we take the magnetic field to be of the form

$$\mathbf{B}(q) = \big(0,0,b(q_1)\big) = b(q_1)\,e_3$$

where $b \in \mathcal{C}^\infty(\mathbb{R})$, and thus $\nabla_q\cdot\mathbf{B} = 0$, $\nabla_q\mathbf{B}_j = 0$ for $j = 1,2$ and $\nabla_q\mathbf{B}_3 = b'\,e_1$. It is easy to solve the equations of motion

$$\dot{q} = p$$
$$\dot{p} = \varepsilon\,\tfrac{\sqrt{3}}{2}\nabla_q\big(\mathbf{B}\cdot n\big) = \varepsilon\,\tfrac{\sqrt{3}}{2}b'\,n_3\,e_1 = \mathcal{O}(\varepsilon) \qquad (5.2)$$
$$\dot{n} = b\,e_3\wedge n$$

explicitly up to $\mathcal{O}(\varepsilon^2)$: the leading-order flow on $\mathbb{R}^6\times\mathbb{S}^2$ is given by

$$\Phi^0_t(q,p,n) = \begin{pmatrix} q + t\,p \\ p \\ N^0(t,q,p,n) \end{pmatrix}$$

where $N^0(t,q,p,n)$ solves

$$\dot{N}^0(t,q,p,n) = b(q_1 + t\,p_1)\,e_3\wedge N^0(t,q,p,n), \qquad N^0(0,q,p,n) = n.$$

Note that the spin precesses around the e_3-axis and thus $N^0_3(t,q,p,n) = n_3$. The flow which solves (5.2) can be found up to $\mathcal{O}(\varepsilon^2)$ by iteration: $\ddot{q} = \varepsilon\,\tfrac{\sqrt{3}}{2}b'(q_1)\,n_3\,e_1$ and hence, for initial momenta $p = (0,p_2,p_3)$ in the p_2p_3-plane, we compute

$$q^\varepsilon(t,q,p,n) = q + t\,p + \varepsilon\,t^2\,\tfrac{\sqrt{3}}{2}\,b'(q_1)\,n_3\,e_1.$$

Thus, classical trajectories starting at (q,p) split into a whole fan of possible directions depending on $n_3 \in [-1,+1]$. This apparent inconsistency with the

quantum mechanical predictions disappears after averaging over an initial distribution of spin. Let us assume for simplicity that the initial state is a product state, $\hat{w} = \hat{w}_{\mathbb{R}^6} \otimes \hat{w}_{\mathbb{S}^2}$, with symbol $w(q, p, n) = w_{\mathbb{R}^6}(q, p)\, w_{\mathbb{S}^2}(n)$. The fact that $w_{\mathbb{S}^2}(n) = \frac{1}{2}\left(\mathfrak{s}_0 + \sqrt{3}\,\mathfrak{s}\cdot n\right)$ is the symbol of a density matrix, i.e.

$$\mathrm{Op}_{\mathbb{S}^2}(w_{\mathbb{S}^2}) = \mathrm{Op}_{\mathbb{S}^2}(w_{\mathbb{S}^2})^*, \quad 0 \le \mathrm{Op}_{\mathbb{S}^2}(w_{\mathbb{S}^2}) \le 1, \quad \mathrm{Tr}_{\mathbb{C}^2}\left(\mathrm{Op}_{\mathbb{S}^2}(w_{\mathbb{S}^2})\right) = 1,$$

implies $\mathfrak{s}_0 = 1$, $\mathfrak{s} \in \mathbb{R}^3$ and $|\mathfrak{s}| \le 1$. The pure states have "spin-direction" $\mathfrak{s} \in \mathbb{S}^2$, while the completely unpolarized state is $w_{\mathbb{S}^2}^0(n) = \frac{1}{2}$. Taking the spin-average of the e_1-deflection

$$\Delta q_1^\varepsilon(t) := q_1^\varepsilon(t) - q_1 = \varepsilon\, t^2\, \tfrac{\sqrt{3}}{2}\, b'(q_1)\, n_3$$

for initial momenta $p = (0, p_2, p_3)$ with respect to $\mathrm{Op}_{\mathbb{S}^2}(w_{\mathbb{S}^2}) = \frac{1}{2}\left(\mathbb{1}_{\mathbb{C}^2} + \mathfrak{s}\cdot\sigma\right)$ yields

$$\mathbb{E}_{w_{\mathbb{S}^2}}\left(\Delta q_1^\varepsilon(t)\right) := \mathrm{Tr}_{\mathbb{C}^2}\left(\mathrm{Op}_{\mathbb{S}^2}\left(\Delta q_1^\varepsilon(t)\right)\mathrm{Op}_{\mathbb{S}^2}(w_{\mathbb{S}^2})\right)$$

$$= \varepsilon\, t^2\, \frac{b'(q_1)}{2}\, \mathrm{Tr}_{\mathbb{C}^2}\left(\sigma_3\, \mathrm{Op}_{\mathbb{S}^2}(w_{\mathbb{S}^2})\right)$$

$$= \varepsilon\, t^2\, \frac{b'(q_1)}{2}\, \mathfrak{s}_3. \tag{5.3}$$

To conclude that the distribution of $\Delta q_1^\varepsilon(t)$ is concentrated in two points, we need to compute higher moments of $\Delta q_1^\varepsilon(t)$. To this end, note that

$$\left(\mathrm{Op}_{\mathbb{S}^2}\left(\Delta q_1^\varepsilon(t)\right)\right)^{2m} = \left(\varepsilon\, t^2\, \frac{|b'(q_1)|}{2}\right)^{2m}\sigma_3^{2m} = \left(\varepsilon\, t^2\, \frac{|b'(q_1)|}{2}\right)^{2m}\mathbb{1}_{\mathbb{C}^2}$$

and

$$\left(\mathrm{Op}_{\mathbb{S}^2}\left(\Delta q_1^\varepsilon(t)\right)\right)^{2m+1} = \left(\varepsilon\, t^2\, \frac{|b'(q_1)|}{2}\right)^{2m+1}$$

$$\sigma_3^{2m+1} = \left(\varepsilon\, t^2\, \frac{|b'(q_1)|}{2}\right)^{2m+1}\sigma_3.$$

Hence,

$$\mathbb{E}_{w_{\mathbb{S}^2}}\left(\left(\Delta q_1^\varepsilon(t)\right)^{2m}\right) = \left(\varepsilon\, t^2\, \frac{|b'(q_1)|}{2}\right)^{2m}$$

and

$$\mathbb{E}_{w_{\mathbb{S}^2}}\left(\left(\Delta q_1^\varepsilon(t)\right)^{2m+1}\right) = \left(\varepsilon\, t^2\, \frac{|b'(q_1)|}{2}\right)^{2m+1}\mathfrak{s}_3.$$

This computation shows how a continuous distribution of classical trajectories in $\mathbb{R}^6 \times \mathbb{S}^2$ leads to a distribution concentrated in two points $\pm\varepsilon\, t^2\, \frac{b'(q_1)}{2}$ with weights $\frac{1}{2}(1 \pm \mathfrak{s}_3)$ after averaging against a spin Wigner function $w_{\mathbb{S}^2}$. Since $w_{\mathbb{S}^2}$ is always equivalent to a linear polynomial, $\mathcal{P}w_{\mathbb{S}^2}(n) = \frac{1}{2}\left(1 + \sqrt{3}\,\mathfrak{s}\cdot n\right)$ is never concentrated around a point on $\mathbb{S}^2$ and takes negative values in case $|\mathfrak{s}| \ge 1/\sqrt{3}$ is large enough.

Of course, we still need to average over an initial distribution $w_{\mathbb{R}^6}(q, p)$ of position and momenta. According to the uncertainty relation, we can assume

that the width of the initial position distribution is $\Delta q_0 = \mathcal{O}(\varepsilon^{1/3})$ and the width of the initial momentum distribution is $\Delta p_0 = \mathcal{O}(\varepsilon^{2/3})$. After time $t \propto \varepsilon^{-1/2}$, the width $\Delta q = \Delta q_0 + t\Delta p_0 = \mathcal{O}(\varepsilon^{1/6})$ of wave packets following the classical trajectories is smaller than the separation $\varepsilon\, t^2\, b'(q_1) = \mathcal{O}(1)$ of the trajectories due to the deflection by the inhomogeneous field.

In conclusion, we see that the semiclassical model can correctly reproduce the splitting of wave packets in inhomogeneous magnetic fields. For the particular case where $b(q_1) = q_1$ is linear and initial momenta $p = (0, p_2, p_3)$ lie in the $p_2 p_3$-plane, we arrive at an effectively one-dimensional problem. Thus, Theorem 3.3 applies and we obtain a semiclassical limit for times of order up to $O(\varepsilon^{-\gamma})$, $\gamma < 1/2$, for suitable observables which are initially independent of n. Hence, we even have a rigorous proof that the semiclassical predictions agree at leading order with the quantum mechanical distributions up to times where the splitting is visible.

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