ULM-TP/04-3
March 2004

Semiclassical propagation of coherent states with spin-orbit interaction

Jens Bolte[1] and Rainer Glaser[2]

Abteilung Theoretische Physik
Universität Ulm, Albert-Einstein-Allee 11
D-89069 Ulm, Germany

Abstract

We study semiclassical approximations to the time evolution of coherent states for general spin-orbit coupling problems in two different semiclassical scenarios: The limit $\hbar \to 0$ is first taken with fixed spin quantum number s and then with $\hbar s$ held constant. In these two cases different classical spin-orbit dynamics emerge. We prove that a coherent state propagated with a suitable classical dynamics approximates the quantum time evolution up to an error of size $\sqrt{\hbar}$ and identify an Ehrenfest time scale. Subsequently an improvement of the semiclassical error to an arbitray order $\hbar^{N/2}$ is achieved by a suitable deformation of the state that is propagated classically.

[1]E-mail address: `jens.bolte@physik.uni-ulm.de`
[2]E-mail address: `rainer.glaser@physik.uni-ulm.de`

1 Introduction

Ever since their introduction by Schrödinger as early as 1926 [Sch26], coherent states have found an increasing range of applications in quantum mechanics, see e.g. [KS85, Per86]. In a semiclassical context their virtues become particularly transparent in attempts to relate the quantum time evolution of a system to its classical trajectories. Coherent states can, e.g., even be used to identify the limiting classical dynamics of a given quantum system.

However, apart from the exceptional case of the harmonic oscillator that Schrödinger chose for his construction, every quantum wave packet necessarily disperses. Schrödinger's original intention to mimic classical trajectories in quantum mechanics can therefore only be put into practice up to the time scale on which wave packets begin to delocalise. Beyond that the quantum time evolution looses its tight relation to classical trajectories, although coarser classical structures possibly remain to be of influence [SB02, Sch04].

More recently the notion of an *Ehrenfest time* was introduced [Chi79, Zas81], intended to indicate that the Ehrenfest relations can only connect quantum dynamics and classical trajectories on limited time scales. For classical dynamics with positive Lyapunov exponents it is argued that the Ehrenfest time is logarithmic in $\hbar$. This conclusion can be drawn from the observation that coherent states are localised in phase space on a scale of $\sqrt{\hbar}$, and that an unstable classical dynamics expands domains in phase space with exponential rates in the unstable directions. Thus for times beyond $\frac{1}{2\lambda}|\log\hbar|$ a coherent state is no longer localised in directions that are expanded with an exponent λ. A finer analysis reveals that the precise value of the Ehrenfest time depends on the problem that is studied; e.g., using L^2-norms to measure the difference between the quantum time evolution of a coherent state and a coherent state that is propagated with the classical dynamics, a critical time scale of $\frac{1}{6\lambda}|\log\hbar|$ was proven to hold [CR97]. On the other hand, the same difference measured in terms of expectation values of observables can be controlled up to times of the order of $\frac{1}{2\lambda}|\log\hbar|$. For details see [CR97, BB00, BR02]. It can moreover be shown that on finite time intervals a coherent state is exponentially localised around the corresponding classical trajectory [HJ00].

Except for heat kernel asymptotics in the case of particles in non-abelian gauge fields [HPS83] most of the previous work on a semiclassical control of the propagation of coherent states is concerned with systems that possess only translational degrees of freedom. In this article it is our aim to extend these investigations to systems with non-relativistic spin-orbit interactions. After having identified appropriate coherent states, we intend to compare solutions of the Schrödinger equation

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

where the initial wave function $\psi(0)$ is a coherent state, with a coherent state that is evolved along suitable classical trajectories. The quantum Hamiltonians that we wish to allow are of a general spin-orbit coupling type,

$$\hat{H} = H_0(\hat{Q},\hat{P}) + \boldsymbol{C}(\hat{Q},\hat{P})\cdot\hat{\boldsymbol{S}} \ , \qquad (1.1)$$

with $\hat{Q}$, $\hat{P}$, and $\hat{\boldsymbol{S}}$ denoting the standard position, momentum, and spin operators, respectively. Examples of such Hamiltonians arise when the spin is coupled to an external magnetic field, such that $\boldsymbol{C} = \frac{e}{mc}\boldsymbol{B}$, or in the context of atomic spin-orbit coupling with $\boldsymbol{C}$ being proportional to orbital angular momentum.

Apart from atomic and molecular physics spin-orbit coupling also plays an important role in nuclei, where it essentially determines their shell structure [BM69], as well as in solid state physics. In the latter case recent experimental progress towards controlling the spin dynamics of electrons in semiconductors [SFHŽ01] calls for a theoretical description of such set-ups. As opposed to some pure quantum calculations semiclassical considerations are often particularly transparent and provide a clear physical picture. With our work we therefore intend to improve the understanding of spin-orbit coupling by establishing mathematically rigorous statements about the quantum dynamics of localised particles with spin and their relation to appropriate classical trajectories.

One issue to be settled is how the semiclassical limit should be performed in the presence of spin-orbit interactions. In principle two parameters controlling the passage to a classical description are available, which are associated with the two types of degrees of freedom: translational and spin. On the one hand, with (an effective) $\hbar$ approaching zero the semiclassical limit is achieved in a standard way for the translational degrees of freedom. On the other hand, for an isolated spin $\hbar$ can be eliminated from both kinematics and dynamics. The role of a semiclassical parameter is then taken over by $1/s$, where $s = 1/2, 1, 3/2, \dots$ denotes the spin quantum number. When both types of degrees of freedom interact through a spin-orbit coupling one can therefore pass to the semiclassical limit in various ways. In the absence of a theory that is uniform in both $\hbar$ and $1/s$ we subsequently focus on two important scenarios:

The most straight forward approach is to view, say, an electron as a particle with fixed spin $1/2$ and to employ $\hbar$ as the only semiclassical parameter. In the limit $\hbar \to 0$ the energy scale of the translational part $\hat{H}_0$ in (1.1) then dominates that of the spin-orbit coupling term, since in the latter the spin operator $\hat{\boldsymbol{S}}$ is proportional to $\hbar$. Although it might appear that thus the spin has evaded the leading order semiclassical description, it does in fact contribute in an essential way through a classical spin precession driven by the orbital motion, see [BK99a, BG00, BGK01, BG04]. E.g., in classically chaotic systems this type of spin motion is responsible for the quantum eigenvalue spectrum to possess correlations of the Gaussian symplectic ensemble of random matrix theory [BK99b]. Moreover, in this semiclassical framework the exact spectrum of the relativistic hydrogen atom is recovered [Kep03], and anomalous magneto-oscillations in semiconductor devices can be described to a good approximation [KW02].

A second option for the semiclassical limit is to keep the "classical spin" $\hbar s$ at a fixed value S, thus performing $\hbar \to 0$ and $s \to \infty$ simultaneously. In this scenario the energy scale of spin-orbit interactions remains comparable to that of the purely translational part, leading to a classical spin-orbit Hamiltonian. Therefore, coupled Hamiltonian dynamics emerge with classical particle trajectories influenced by the spin. This scenario enables an immediate classical description of the Stern-Gerlach experiment, and generally corresponds to a "strong" spin-orbit coupling.

In this paper we examine the propagation of coherent states under the influence of spin-orbit interactions in both of the above mentioned semiclassical scenarios. In section 2 we first provide a precise characterisation of the quantum Hamiltonians under investigation and then describe the classical dynamics that will result in due course. Section 3 is devoted to outlining the construction of coherent states for both translational and spin degrees of freedom, along with their basic properties. Our principal results are developed in section 4. For both semiclassical scenarios separately we extend the approach devised previously [Hel75, Lit86, CR97] in systems without spin in that we first construct suitable approximate Hamiltonians that propagate coherent states exactly along classical trajectories. We then prove that, measured in Hilbert space norm, the full quantum dynamics differs from a classically propagated coherent states by an error of size $\sqrt{\hbar}$ as long as finite times are taken into account. The vanishing of this difference up to some, semiclassically infinite, Ehrenfest time is also established. Subsequently we improve the semiclassical error to $O(\hbar^{N/2})$ for arbitrary $N \in \mathbb{N}$ by replacing the classically propagated coherent states with a suitable sum of squeezed states. Again such a procedure is possible up to the Ehrenfest time. We conclude in section 5 with discussing some implications of our main results.

2 Background

It is our aim to investigate the time evolution of an initial coherent state in both translational and spin degrees of freedom generated by a general spin-orbit quantum Hamiltonian with an emphasis on a semiclassical description. This is the reason why we represent quantum observables as matrix valued semiclassical pseudodifferential operators within the framework of Weyl calculus, see [Rob87, DS99] for details. The quantum Hamiltonians $\hat{H}$ under consideration are defined on the domain $\mathscr{S}(\mathbb{R}^d) \otimes \mathbb{C}^{2s+1}$ in the Hilbert space $L^2(\mathbb{R}^d) \otimes \mathbb{C}^{2s+1}$ and are of the form

$$\big(\hat{H}\psi\big)(x) = \big(\mathrm{op}^W[H]\psi\big)(x) = \frac{1}{(2\pi\hbar)^d} \iint_{\mathrm{T}^*\mathbb{R}^d} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\xi\cdot(x-y)}\, H\Big(\frac{x+y}{2},\xi\Big)\, \psi(y)\; \mathrm{d}y\, \mathrm{d}\xi \; . \tag{2.1}$$

Here $\mathrm{T}^*\mathbb{R}^d \cong \mathbb{R}^d \times \mathbb{R}^d$ denotes the cotangent bundle over the euclidean configuration space $\mathbb{R}^d$, i.e. the phase space of the translational degrees of freedom. The spin $s = 1/2, 1, 3/2, \dots$ is described by the matrix degrees of freedom of the Weyl symbol H and will later be represented on its phase space S^2. Spin-orbit Hamiltonians are characterised by symbols of the form

$$H(x,\xi) = H_0(x,\xi) + \hbar\, \boldsymbol{C}(x,\xi) \cdot \mathrm{d}\pi_s(\boldsymbol{\sigma}/2) \;, \tag{2.2}$$

where H_0 and the components C_k, $k = 1,2,3$, of $\boldsymbol{C}$ are real valued and smooth functions on $\mathrm{T}^*\mathbb{R}^d$ which for all multi-indices α and β satisfy the growth estimate

$$|\partial_x^\alpha \partial_\xi^\beta F(x,\xi)| \leq K_{\alpha\beta}\, \big(1+|x|^2\big)^{M_x/2} \big(1+|\xi|^2\big)^{M_\xi/2} \tag{2.3}$$

with suitable constants $K_{\alpha\beta} > 0$ and $M = (M_x, M_\xi) \in \mathbb{R}^2$.

The spin-orbit coupling term in (2.2) contains the spin operators

$$\hat{S}_k := \hbar\, \mathrm{d}\pi_s(\sigma_k/2)\ , \qquad k = 1,2,3\ ,$$

obeying the well known commutation relations $[\hat{S}_k, \hat{S}_l] = \mathrm{i}\hbar\, \epsilon_{klm}\, \hat{S}_m$. Here

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\ , \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}\ , \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.4}$$

are the Pauli matrices, considered as elements of the real Lie algebra su(2), and $\mathrm{d}\pi_s$ denotes the $(2s{+}1)$-dimensional representation of su(2) derived from the corresponding unitary irreducible representation π_s of the Lie group SU(2) according to $\mathrm{d}\pi_s(X) = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\lambda}\, \pi_s\big(\mathrm{e}^{-\mathrm{i}\lambda X}\big)\big|_{\lambda=0}$.

The time evolution $\hat{U}(t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}$ generated by the quantum Hamiltonian will be unitary provided that $\hat{H}$ itself is essentially self-adjoint on the domain $C_0^\infty(\mathbb{R}^d) \otimes \mathbb{C}^{2s+1}$. In the present framework this is guaranteed, for sufficiently small $\hbar$, once the symbol H is such that $H + \mathrm{i}$ is elliptic, i.e. if

$$\big\| \big(H(x,\xi) + \mathrm{i}\big)^{-1} \big\| \leq c\, \big(1 + |x|^2\big)^{-M_x/2} \big(1 + |\xi|^2\big)^{-M_\xi/2} \tag{2.5}$$

holds for all $(x,\xi) \in \mathrm{T}^*\mathbb{R}^d$ with some constant $c > 0$ and M as in (2.3); here $\|\cdot\|$ is an arbitrary matrix norm. Details can be found in [Rob87, DS99]. In the following we assume this condition to hold and do not notationally distinguish between $\hat{H}$ and its self-adjoint extension.

In the semiclassical limit we will have to deal with two types of classical spin-orbit dynamics. In the first case only the translational degrees of freedom evolve under a Hamiltonian flow. This is defined on the phase space $\mathrm{T}^*\mathbb{R}^d$ and is generated by the classical Hamiltonian H_0. Thus $\Phi_0^t(q,p) = \big(q(t), p(t)\big)$ satisfies Hamilton's equations of motion,

$$\dot{q}(t) = \partial_\xi H_0\big(q(t), p(t)\big) \quad \text{and} \quad \dot{p}(t) = -\partial_x H_0\big(q(t), p(t)\big)\ ,$$

with initial conditions $\big(q(0), p(0)\big) = (q,p)$. This flow then drives a classical spin through the equations of motion

$$\dot{\boldsymbol{n}}(t) = \boldsymbol{C}\big(q(t), p(t)\big) \times \boldsymbol{n}(t)$$

on the sphere S^2 with initial condition $\boldsymbol{n}(0) = \boldsymbol{n}$. Here $\boldsymbol{n} \in \mathbb{R}^3$ with $|\boldsymbol{n}| = 1$ is considered as a point on S^2. The curve $\boldsymbol{n}(t)$ therefore describes the Thomas precession of a normalised classical spin vector on S^2 along the trajectory $\big(q(t), p(t)\big)$ in $\mathrm{T}^*\mathbb{R}^d$. The combined dynamics

$$(q, p, \boldsymbol{n}) \mapsto \big(\Phi_0^t(q,p), \boldsymbol{n}(t; q, p, \boldsymbol{n})\big) \tag{2.6}$$

yield a flow on the product phase space $\mathrm{T}^*\mathbb{R}^d \times \mathrm{S}^2$, which is a symplectic manifold whose symplectic form is composed of the natural symplectic forms of its factors. This flow has the form of a skew product, see [CFS82] for details, and thus is not Hamiltonian; however, it leaves the natural volume measure derived from the symplectic form invariant.

The second flow relevant for our subsequent discussion includes a classical spin dynamics coupled to the motion of the translational part in a Hamiltonian manner and is also defined on the product phase space $\mathrm{T}^*\mathbb{R}^d \times \mathrm{S}^2$. These dynamics are generated by the classical spin-orbit Hamiltonian

$$H_{\mathrm{so}}(x,\xi,\boldsymbol{n}) := H_0(x,\xi) + S\boldsymbol{n}\cdot\boldsymbol{C}(x,\xi)\ , \tag{2.7}$$

where the constant $S>0$ measures the length of the classical spin vector $\boldsymbol{s} := S\boldsymbol{n}$. The Hamiltonian flow $\Phi^t_{\mathrm{so}}(q,p,\boldsymbol{n}) = \big(q(t),p(t),\boldsymbol{n}(t)\big)$ is therefore determined by the equations of motion

$$\begin{aligned}\dot q(t) &= \partial_\xi H_{\mathrm{so}}\big(q(t),p(t),\boldsymbol{n}(t)\big)\ ,\\ \dot p(t) &= -\partial_x H_{\mathrm{so}}\big(q(t),p(t),\boldsymbol{n}(t)\big)\ ,\\ \dot{\boldsymbol{n}}(t) &= \boldsymbol{C}\big(q(t),p(t)\big)\times\boldsymbol{n}(t)\ .\end{aligned} \tag{2.8}$$

The Hamiltonian coupling of the degrees of freedom prescribed by these equations imply that in contrast to the previous case the translational dynamics are affected by the spin.

Apart from the associated classical flow in semiclassical approximations of quantum dynamics also the linear stability of the flow plays a role. Quantitatively this can be measured in terms of the Lyapunov exponents, see the appendix for a discussion. They express the rate of phase space expansion or contraction, respectively, induced by the flow in different tangent directions. Moreover, the differential of the flow is a symplectic map on the tangent bundle of phase space. Its metaplectic representation is an essential ingredient in the semiclassical propagation of coherent states.

3 Coherent states

Within the setting outlined in the preceding section we wish to describe the time evolution of an initial coherent state semiclassically. The starting point therefore is the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t}(t,x) = \hat H\psi(t,x) \qquad \text{with} \qquad \psi(0,x) = \big(\varphi^B_{(q,p)}\otimes\phi_{\boldsymbol{n}}\big)(x)\ ,$$

whose initial condition is the product of a coherent state $\varphi^B_{(q,p)}$ of the translational degrees of freedom and a spin-coherent state $\phi_{\boldsymbol{n}}$. The principal question we then address is to what extent the quantum mechanical time evolution can be approximated by some classical dynamics, i.e. we want to estimate the difference

$$\Big\|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat H t}\big(\varphi^B_{(q,p)}\otimes\phi_{\boldsymbol{n}}\big) - \mathrm{e}^{\mathrm{i}\alpha(t)}\,\varphi^{B(t)}_{(q(t),p(t))}\otimes\phi_{\boldsymbol{n}(t)}\Big\| \tag{3.1}$$

in terms of $\hbar$, where $\big(q(t),p(t),\boldsymbol{n}(t)\big)$ is an appropriate classical trajectory and $\mathrm{e}^{\mathrm{i}\alpha(t)}$ is a suitable phase factor.

For both types of coherent states, $\varphi^B_{(q,p)}\in L^2(\mathbb{R}^d)$ and $\phi_{\boldsymbol{n}}\in\mathbb{C}^{2s+1}$, we use Perelomov's construction [Per86] that applies to a general Lie group G with unitary irreducible representation π on a Hilbert space $\mathcal{H}$: Fix a non-zero vector $\Psi_0\in\mathcal{H}$ and consider $\Psi_g := \pi(g)\Psi_0$ for every $g\in G$. Hence the vectors Ψ_g and Ψ_h define the same quantum state, i.e. $\Psi_h = \mathrm{e}^{\mathrm{i}\alpha}\Psi_g$, if and only if $g^{-1}h$ lies in the stability subgroup $H\subset G$ of the vector Ψ_0,

$$H := \{g\in G;\ \pi(g)\Psi_0 = \mathrm{e}^{\mathrm{i}\alpha(g)}\Psi_0\}\ . \tag{3.2}$$

The quantum states generated by the vectors Ψ_g, $g \in G$, can thus be labeled by the points η of the coset space G/H. A section $g(\eta)$ in the bundle $G \to G/H$ then determines a choice of vectors

$$\Phi_\eta := \Psi_{g(\eta)} = \pi(g(\eta))\Psi_0 \ , \qquad \text{for } \eta \in G/H \ , \tag{3.3}$$

representing these states. The vectors Φ_η are called coherent state vectors for $(G, \pi, \mathcal{H})$.

The two types of coherent states that play a role in the present setting can be constructed according to this general scheme by choosing the Heisenberg group $G = H(\mathbb{R}^d)$ for the translational part and the group $G = \mathrm{SU}(2)$ for the spin part. We now describe the two situations that emerge from this procedure separately.

3.1 Coherent states for the Heisenberg group

The Heisenberg group $H(\mathbb{R}^d)$ is a non-compact $(2d+1)$-dimensional Lie group that consists of the elements (q, p, λ) with $(q, p) \in \mathrm{T}^*\mathbb{R}^d$ and $\lambda \in \mathbb{R}$. The group multiplication is given by

$$(q, p, \lambda)\,(q', p', \lambda') = \big(q + q', p + p', \lambda + \lambda' + \tfrac{1}{2}(pq' - qp')\big) \ .$$

According to the Stone-von Neumann Theorem any unitary irreducible representation π of $H(\mathbb{R}^d)$ that fulfills $\pi(0, 0, \lambda) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\lambda}$ is unitarily equivalent to the Schrödinger representation $\rho_\hbar$ on $L^2(\mathbb{R}^d)$,

$$\big(\rho_\hbar(q, p, \lambda)\psi\big)(x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\lambda}\,\big(\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(p\hat{Q} - q\hat{P})}\psi\big)(x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\lambda + p(x - \frac{1}{2}q))}\,\psi(x - q) \ .$$

Here $\hat{Q}_k$ and $\hat{P}_k$, $k = 1, \ldots, d$, are the standard self-adjoint position and momentum operators defined on suitable domains in $L^2(\mathbb{R}^d)$.

In order to construct coherent states for the Heisenberg group we therefore consider the Schrödinger representation $\rho_\hbar$ on $L^2(\mathbb{R}^d)$. One immediately sees that given any non-zero vector $\Psi_0 \in L^2(\mathbb{R}^d)$ its stability subgroup is $H = \{(0, 0, \lambda);\ \lambda \in \mathbb{R}\}$. Thus coherent states can be labeled by points $(q, p) \in G/H$, i.e. by points in the phase space $\mathrm{T}^*\mathbb{R}^d$. This labeling can be achieved in terms of the section $g(q, p) := (q, p, -\frac{1}{2}qp)$ in $G \to G/H$. One usually prefers a reference vector $\Psi_0 \in L^2(\mathbb{R}^d)$ that is normalised, rapidly decreasing, and satisfies

$$\langle \Psi_0, \hat{Q}\Psi_0\rangle = 0 \qquad \text{and} \qquad \langle \Psi_0, \hat{P}\Psi_0\rangle = 0 \ ,$$

so that any reasonable lift of this vector to the phase space $\mathrm{T}^*\mathbb{R}^d$ is concentrated at $(0, 0) \in \mathrm{T}^*\mathbb{R}^d$. A convenient choice with these properties is

$$\psi_0^B(x) := \frac{1}{(\pi\hbar)^{d/4}}\,(\det \operatorname{Im} B)^{1/4}\,\mathrm{e}^{\frac{\mathrm{i}}{2\hbar}xBx} \ ,$$

where B is some complex symmetric $d \times d$ matrix with positive-definite imaginary part. The coherent states (3.3) that follow from the above definitions now read

$$\begin{aligned} \varphi^B_{(q,p)}(x) &= \big(\rho_\hbar(q, p, -\tfrac{1}{2}qp)\psi_0^B\big)(x) \\ &= \frac{1}{(\pi\hbar)^{d/4}}\,(\det \operatorname{Im} B)^{1/4}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left(p(x-q) + \frac{1}{2}(x-q)B(x-q)\right)} \ . \end{aligned} \tag{3.4}$$

Note that these coherent states differ slightly from more conventional choices for which $B = \mathrm{i}\mathbb{1}_d$ and the section $\tilde{g}(q,p) = (q,p,0)$ are used, leading to a different phase convention. Despite the fact that after allowing for more general matrices B the coherent states loose the minimum uncertainty property, this generalisation will prove useful since the action of the metaplectic representation on them can be conveniently expressed in terms of B, see also [Sch01]. The alternative phase convention is of less consequence but simplifies the notation.

Although from the above construction it is obvious that a coherent state $\varphi^B_{(q,p)}$ is concentrated in some neighbourhood of the point (q,p) in phase space it is instructive to calculate explicit phase-space lifts. E.g., its Wigner transform is given by

$$\begin{aligned} W[\varphi^B_{(q,p)}](x,\xi) &= \int_{\mathbb{R}^d} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\xi y}\, \overline{\varphi^B_{(q,p)}(x-\tfrac{1}{2}y)}\, \varphi^B_{(q,p)}(x+\tfrac{1}{2}y)\, \mathrm{d}y \\ &= 2^d\, \mathrm{e}^{-\frac{1}{\hbar}((x,\xi)-(q,p))G_B((x,\xi)-(q,p))}\ , \end{aligned} \tag{3.5}$$

where G_B is the positive-definite symmetric $2d \times 2d$ matrix

$$G_B := \begin{pmatrix} \operatorname{Im} B + \operatorname{Re} B(\operatorname{Im} B)^{-1} \operatorname{Re} B & -\operatorname{Re} B(\operatorname{Im} B)^{-1} \\ -(\operatorname{Im} B)^{-1} \operatorname{Re} B & (\operatorname{Im} B)^{-1} \end{pmatrix} .$$

This representation reveals a concentration of the coherent state in the vicinity of the phase-space point (q,p). Moreover, since the sum of position and momentum uncertainties reads

$$\frac{1}{(2\pi\hbar)^d} \iint_{\mathrm{T}^*\mathbb{R}^d} \big((x-q)^2 + (\xi-p)^2\big)\, W[\varphi^B_{(q,p)}](x,\xi)\, \mathrm{d}x\, \mathrm{d}\xi = \frac{\hbar}{2}\big(\operatorname{tr} G_B\big)^{-1}\ , \tag{3.6}$$

the spreading of the coherent state in phase space can be measured in terms of G_B.

3.2 Spin-coherent states

In quantum mechanics the spin of a particle is implemented through the $(2s+1)$-dimensional irreducible representation π_s of the compact Lie group SU(2), where $s = 1/2, 1, 3/2, \ldots$ denotes the spin quantum number. Within Perelomov's framework spin-coherent states are hence constructed from $(\mathrm{SU}(2), \pi_s, \mathbb{C}^{2s+1})$. The reference vector $\Psi_0 \in \mathbb{C}^{2s+1}$ can be chosen such that the coherent states possess the minimum uncertainty property; this is achieved with Ψ_0 being a maximal weight vector for the irreducible representation $\mathrm{d}\pi_s$ of the Lie algebra su(2).

The real Lie algebra su(2) consists of the hermitian and traceless 2×2 matrices X, such that $\mathrm{e}^{-\mathrm{i}X} \in \mathrm{SU}(2)$. A convenient basis of su(2) is formed by the Pauli matrices (2.4). We also consider the complexified Lie algebra $\mathrm{su}(2)_{\mathbb{C}} := \mathrm{su}(2) \otimes \mathbb{C}$ with basis given by

$$X_\pm := \frac{1}{2}(\sigma_1 \pm \mathrm{i}\sigma_2)\ , \quad X_3 := \frac{1}{2}\sigma_3\ ,$$

and commutation relations

$$[X_3, X_\pm] = \pm X_\pm \ , \quad [X_+, X_-] = 2X_3 \ .$$

The vector X_3 spans a Cartan subalgebra, which exponentiates to a maximal torus $T \simeq \mathrm{U}(1)$ in SU(2), and $X_\pm \in \mathrm{su}(2)_\mathbb{C}$ span the root spaces $\mathfrak{g}_\pm \subset \mathrm{su}(2)_\mathbb{C}$. Their representations $\mathrm{d}\pi_s(X_\pm)$ are raising and lowering operators, respectively. More precisely, the representation space $\mathbb{C}^{2s+1}$ decomposes into a direct sum of the one dimensional eigenspaces of $\mathrm{d}\pi_s(X_3)$ (weight spaces) $V_m = \{\phi \in \mathbb{C}^{2s+1};\ \mathrm{d}\pi_s(X_3)\phi = m\phi\}$, where $m = -s, -s+1, \dots, s$. The raising and lowering operators $\mathrm{d}\pi_s(X_\pm)$ map the weight spaces into one another, $\mathrm{d}\pi_s(X_\pm)V_m = V_{m\pm1}$ for $m \neq \pm s$. The weights $m = \pm s$ are called maximal and minimal weights, respectively. The corresponding weight vectors are annihilated by the raising or lowering operator. In the usual angular momentum notation a normalised weight vector is denoted as $|s, m\rangle$.

For a given representation π_s of SU(2) we choose a maximal weight vector $|s, s\rangle$ as the reference vector Ψ_0. According to (3.2) the stability group of this vector is

$$H = \{g = \mathrm{e}^{-\mathrm{i}\lambda\sigma_3};\ \lambda \in [0, 2\pi)\} \cong \mathrm{U}(1) \ ,$$

which can be identified with a maximal torus T. Thus coherent states are labeled by points in the coset space

$$G/H \cong \mathrm{SU}(2)/\mathrm{U}(1) \cong \mathrm{S}^2 \ .$$

As in the case of the Heisenberg group this manifold is naturally symplectic and can be viewed as the corresponding classical phase space.

The definition of coherent states finally requires a section in $G \to G/H$, i.e. in the Hopf bundle $\mathrm{SU}(2) \to \mathrm{S}^2$. This principal U(1)-bundle, however, is non-trivial so that no smooth global section exists. We therefore here give local constructions that, nevertheless, allow for suitable interpretations in terms of global objects. We parameterise points on S^2 by $\boldsymbol{n} \in \mathbb{R}^3$ with $|\boldsymbol{n}| = 1$ and use spherical coordinates, $\boldsymbol{n}(\theta, \varphi) = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ with $\theta \in [0, \pi)$ and $\varphi \in [0, 2\pi)$. Introducing $\boldsymbol{e}_\varphi := (-\sin\varphi, \cos\varphi, 0)$ our choice of a local section reads (see also [Per86])

$$g_{\boldsymbol{n}} = \mathrm{e}^{-\frac{\mathrm{i}}{2}\theta \boldsymbol{e}_\varphi \cdot \boldsymbol{\sigma}} = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2}\,\mathrm{e}^{-\mathrm{i}\varphi} \\ \sin\frac{\theta}{2}\,\mathrm{e}^{\mathrm{i}\varphi} & \cos\frac{\theta}{2} \end{pmatrix} \ .$$

Under the double covering map $R : \mathrm{SU}(2) \to \mathrm{SO}(3)$ that is defined through $(R(g)\boldsymbol{x}) \cdot \boldsymbol{\sigma} = g\boldsymbol{x} \cdot \boldsymbol{\sigma} g^{-1}$, the matrix $g_{\boldsymbol{n}(\theta,\varphi)}$ corresponds to the rotation $R(g_{\boldsymbol{n}(\theta,\varphi)})$ about the axis $\boldsymbol{e}_\varphi$ with angle $-\theta$, such that $R(g_{\boldsymbol{n}})\boldsymbol{e}_3 = \boldsymbol{n}$, where $\boldsymbol{e}_3 = (0, 0, 1)$ represents the north pole on S^2. With these choices spin-coherent states are the normalised vectors

$$\phi_{\boldsymbol{n}} := \pi_s(g_{\boldsymbol{n}})|s, s\rangle \ . \tag{3.7}$$

These states are conveniently represented on the phase space S^2 through the Husimi transform (see [Per86]),

$$h[\phi_{\boldsymbol{n}}](\boldsymbol{m}) := |\langle \phi_{\boldsymbol{m}}, \phi_{\boldsymbol{n}} \rangle| = \left(\frac{1 + \boldsymbol{m} \cdot \boldsymbol{n}}{2}\right)^s \ ,$$

which clearly indicates a concentration, in the semiclassical limit $s \to \infty$, of $\phi_{\boldsymbol{n}}$ at the point $\boldsymbol{n} \in \mathrm{S}^2$.

Our next aim is to investigate the relation between the propagation of a spin-coherent state (3.7) generated by a (time-dependent, linear) spin-Hamiltonian

$$\hat{H}_{\mathrm{spin}} = \boldsymbol{C}(t) \cdot \hat{\boldsymbol{S}} \tag{3.8}$$

defined on $\mathbb{C}^{2s+1}$, and a suitable classical time evolution $\boldsymbol{n}(t)$ on S^2. Here $\hat{\boldsymbol{S}}$ denotes the vector of spin operators $\hat{S}_k = \hbar\, \mathrm{d}\pi_s(\sigma_k/2)$. The dynamics of a coherent state $\phi_{\boldsymbol{n}}$ follows from the equation

$$\mathrm{i}\hbar \frac{\partial \phi}{\partial t}(t) = \hat{H}_{\mathrm{spin}} \phi(t) \qquad \text{with} \qquad \phi(0) = \phi_{\boldsymbol{n}} \; . \tag{3.9}$$

A solution of this problem can be related to the curve $g(t)$, $t \in \mathbb{R}$, in SU(2) determined by

$$\dot{g}(t) + \tfrac{\mathrm{i}}{2}\, \boldsymbol{C}(t) \cdot \boldsymbol{\sigma}\, g(t) = 0 \qquad \text{with} \qquad g(0) = \mathrm{id}_{\mathrm{SU}(2)} \tag{3.10}$$

through

$$\phi(t) = \pi_s(g(t))\phi(0) = \pi_s\big(g(t) g_{\boldsymbol{n}}\big)|s,s\rangle \; . \tag{3.11}$$

An associated classical time evolution then arises from the adjoint action of $g(t)$ on $\boldsymbol{n}\cdot\boldsymbol{\sigma} \in$ su(2) via $\boldsymbol{n}(t) \cdot \boldsymbol{\sigma} := g(t) \boldsymbol{n} \cdot \boldsymbol{\sigma} g(t)^{-1} = (R(g(t))\boldsymbol{n}) \cdot \boldsymbol{\sigma}$. This implies

$$\dot{\boldsymbol{n}}(t) = \boldsymbol{C}(t) \times \boldsymbol{n}(t) \qquad \text{with} \qquad \boldsymbol{n}(0) = \boldsymbol{n} \; . \tag{3.12}$$

The corresponding coherent state vector $\phi_{\boldsymbol{n}(t)}$ differs from the quantum time evolution $\phi(t)$ of $\phi_{\boldsymbol{n}}$ only by a phase; both vectors therefore describe the same quantum state.

Since this phase is required for later purposes, we now determine it explicitly. To this end we notice that $\boldsymbol{n}(t)$ can on the one hand be represented as

$$\boldsymbol{n}(t) = R\big(g(t)\big)\boldsymbol{n} = R\big(g(t) g_{\boldsymbol{n}}\big)\boldsymbol{e}_3 \; ,$$

and on the other hand as

$$\boldsymbol{n}(t) = R\big(g_{\boldsymbol{n}(t)}\big)\boldsymbol{e}_3 \; .$$

Thus, under the double covering map, $g_{\boldsymbol{n}(t)}^{-1} g(t) g_{\boldsymbol{n}} \in \mathrm{SU}(2)$ is associated with a rotation about $\boldsymbol{e}_3$ with some angle $\varrho(t)$, such that

$$g_{\boldsymbol{n}(t)}^{-1} g(t) g_{\boldsymbol{n}} = \mathrm{e}^{\frac{\mathrm{i}}{2}\varrho(t)\sigma_3} \in T \; .$$

From (3.11) it now follows that

$$\phi(t) = \pi_s\big(g(t) g_{\boldsymbol{n}}\big)|s,s\rangle = \pi_s\big(g_{\boldsymbol{n}(t)}\big)\pi_s\big(\mathrm{e}^{\frac{\mathrm{i}}{2}\varrho(t)\sigma_3}\big)|s,s\rangle = \mathrm{e}^{\mathrm{i}s\varrho(t)}\, \phi_{\boldsymbol{n}(t)} \; , \tag{3.13}$$

thus confirming the claimed relation between the quantum and 'classical' propagation of the spin-coherent state $\phi_{\boldsymbol{n}}$. Due to the explicit dependence of the phase on s it suffices to calculate the angle $\varrho(t)$ for $s = \frac{1}{2}$. For this one notices that in polar coordinates

$$\phi(t) = \mathrm{e}^{\frac{\mathrm{i}}{2}\varrho(t)}\, g_{\boldsymbol{n}(t)}|\tfrac{1}{2},\tfrac{1}{2}\rangle = \begin{pmatrix} \cos(\frac{\theta(t)}{2})\, \mathrm{e}^{\frac{\mathrm{i}}{2}\varrho(t)} \\ \sin(\frac{\theta(t)}{2})\, \mathrm{e}^{\mathrm{i}(\varphi(t)+\frac{1}{2}\varrho(t))} \end{pmatrix} \; . \tag{3.14}$$

In a standard calculation (see e.g. [BK99b]) $\varrho(t)$ can now be determined by using (3.14) in equation (3.9), leading to

$$\varrho(t) = -\int_0^t \Big(\boldsymbol{C}(t') \cdot \boldsymbol{n}(t') + \big(1 - \cos\theta(t')\big)\dot{\varphi}(t') \Big) \, \mathrm{d}t' \; . \tag{3.15}$$

If one introduces a classical spin vector $\boldsymbol{s} := S\boldsymbol{n}$, with some $S > 0$, one can relate the angle $\varrho(t)$ to Hamilton's principal function of the spin. The observation that

$$L_{\mathrm{spin}}(t) = -\boldsymbol{C}(t) \cdot \boldsymbol{s}(t) - S\,\big(1 - \cos\theta(t)\big)\dot{\varphi}(t)$$

is the Lagrangean of the classical spin motion implies $S\varrho(t)$ to be the spin-action $R_{\mathrm{spin}}(t)$.

4 Time evolution of coherent states

In this section we discuss the time evolution of coherent states in two different semiclassical limits. In the first scenario we consider $\hbar \to 0$ while the spin quantum number s is fixed. This will imply that primarily the translational degrees of freedom become semiclassical. The spin-orbit interaction therefore occurs on the level of the subprincipal symbol of the Hamiltonian (2.2), enforcing the skew-product structure (2.6) of the resulting classical dynamics with the translational motion driving the spin.

In the second scenario we fix the product $S := \hbar s$ and hence consider the combined limits $\hbar \to 0$ and $s \to \infty$. Thus both types of degrees of freedom are treated semiclassically on equal footing. This results in a classical spin-orbit coupling with the Hamiltonian dynamics (2.8) generated by the function (2.7).

We begin with the first scenario which is close to the time evolution of coherent states without spin degrees of freedom.

4.1 Semiclassics with fixed spin

In the present scenario $\hbar$ is the only semiclassical parameter so that we consider the quantum Hamiltonian (2.1) as a Weyl operator with matrix valued symbol (2.2) that has a scalar principal part; the subprincipal symbol then contains the spin-orbit coupling. This setting ensures that the propagation of coherent states is closely analogous to the case without spin, compare [CR97].

Guided by this analogy we first construct an approximate Hamiltonian that propagates coherent states exactly. Regarding the translational part we exploit the fact that the time evolution generated by a quadratic Hamiltonian preserves the form $\varphi^B_{(q,p)}$ given in (3.4) of a coherent state for the Heisenberg group. The spin part of the coherent state shall be propagated by a Hamiltonian of the form (3.8) and can hence be calculated explicitly. Using the convenient notation $w := (x, \xi) \in \mathrm{T}^*\mathbb{R}^d$, we now consider the Taylor expansion of the symbol (2.2) about some smooth curve $z(t) = \big(q(t), p(t)\big)$ in phase space. The Weyl quantisation of the leading terms in the Taylor expansion (of different order in the principal and in the subprincipal symbol),

$$H_Q(t,w) := \sum_{|\nu|=0}^{2} \frac{1}{\nu!} H_0^{(\nu)}\big(z(t)\big)\big(w-z(t)\big)^{\nu} + \hbar\, \boldsymbol{C}\big(z(t)\big)\cdot \mathrm{d}\pi_s(\boldsymbol{\sigma}/2) \ , \tag{4.1}$$

yields a quantum Hamiltonian $\hat{H}_Q(t)$ that is quadratic in $\hat{Q}$ and $\hat{P}$ and linear in $\hat{\boldsymbol{S}}$. Here $H_0^{(\nu)}(w)$ stands for the derivative $\partial_w^\nu H_0(w)$ of order $|\nu|$ in the $2d$ components of $w=(x,\xi)$. The time evolution $\psi_Q(t) \in L^2(\mathbb{R}^d)\otimes\mathbb{C}^{2s+1}$ of a coherent state $\varphi^B_{(q,p)}\otimes\phi_{\boldsymbol{n}}$ generated by the approximate Hamiltonian,

$$\mathrm{i}\hbar \frac{\partial \psi_Q}{\partial t}(t) = \hat{H}_Q(t)\psi_Q(t) \qquad \text{with} \qquad \psi_Q(0) = \varphi^B_{(q,p)}\otimes\phi_{\boldsymbol{n}} \ , \tag{4.2}$$

can be expressed in terms of a coherent state:

Proposition 4.1. *The solution of the quadratic Schrödinger equation (4.2) is a time-dependent coherent state with an additional phase,*

$$\psi_Q(t) = \mathrm{e}^{\mathrm{i}\left(\frac{R_0(t)}{\hbar}+s\varrho(t)+\frac{\pi}{2}\sigma(t)\right)}\, \varphi^{B(t)}_{(q(t),p(t))}\otimes\phi_{\boldsymbol{n}(t)} \ . \tag{4.3}$$

Here $\big(q(t),p(t)\big)=\Phi_0^t(q,p)$ is the solution of Hamilton's equations of motion generated by the principal symbol H_0,

$$\dot{q}(t) = \partial_\xi H_0\big(q(t),p(t)\big) \ , \qquad \dot{p}(t) = -\partial_x H_0\big(q(t),p(t)\big) \ , \tag{4.4}$$

with initial condition $\big(q(0),p(0)\big)=(q,p)$ and principal function

$$R_0(t) = \int_0^t \big(p(t')\dot{q}(t') - H_0(q(t'),p(t'))\big)\ \mathrm{d}t' \ . \tag{4.5}$$

The complex symmetric $d\times d$ matrix $B(t)$ is given by

$$B(t) = \big(\partial_q q(t) B + \partial_p q(t)\big)\big(\partial_q p(t)B+\partial_p p(t)\big)^{-1} \ , \tag{4.6}$$

where the derivatives are taken with respect to the initial conditions; it also gives rise to the Maslov phase $\sigma(t)$. Moreover, $\boldsymbol{n}(t)$ is a solution of the spin precession equation (3.12) in which $\boldsymbol{C}(t)$ stands for $\boldsymbol{C}\big(q(t),p(t)\big)$ from (4.1); $\varrho(t)$ then is the associated angle (3.15).

Proof. For the proof we adapt the method of [Sch01] to the present situation and therefore introduce the ansatz

$$\psi_Q(t,x) = (\pi\hbar)^{-d/4}\,\gamma(t)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\theta(t)}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left(p(t)(x-q(t))+\frac{1}{2}(x-q(t))B(t)(x-q(t))\right)}\,\phi_{\boldsymbol{n}(t)}$$

in equation (4.2). To deal with the spin contribution to the left-hand side we use the fact that according to (3.9) and (3.13)

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\big(\mathrm{e}^{\mathrm{i}s\varrho(t)}\,\phi_{\boldsymbol{n}(t)}\big) = \hbar\,\boldsymbol{C}\big(q(t),p(t)\big)\cdot\mathrm{d}\pi_s(\boldsymbol{\sigma}/2)\,\mathrm{e}^{\mathrm{i}s\varrho(t)}\,\phi_{\boldsymbol{n}(t)} \ , \tag{4.7}$$

if and only if $\boldsymbol{n}(t)$ solves (3.12). It hence remains to consider (see [Sch01])

$$
\begin{aligned}
\mathrm{i}\hbar\frac{\partial}{\partial t}&\Big((\pi\hbar)^{-d/4}\,\gamma(t)\,\mathrm{e}^{\mathrm{i}\left(\frac{\theta(t)}{\hbar}-s\varrho(t)\right)}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left(p(t)(x-q(t))+\frac{1}{2}(x-q(t))B(t)(x-q(t))\right)}\Big)\,\mathrm{e}^{\mathrm{i}s\varrho(t)}\,\phi_{\boldsymbol{n}(t)}\\
&=\Big[H_0+H'_{0,x}(x-q(t))+H'_{0,\xi}\cdot B(t)(x-q(t))+\frac{1}{2}(x-q(t))\cdot H''_{0,xx}(x-q(t))\\
&\quad+\frac{1}{2}(x-q(t))\cdot H''_{0,\xi x}B(t)(x-q(t))+\frac{1}{2}(x-q(t))\cdot B(t)H''_{0,\xi x}(x-q(t))\\
&\quad+\frac{1}{2}(x-q(t))\cdot B(t)H''_{0,\xi\xi}B(t)(x-q(t))+\frac{\hbar}{2\mathrm{i}}\,\mathrm{tr}\big(H''_{0,\xi x}+H''_{0,\xi\xi}B(t)\big)\Big]\;\psi_Q(t,x)\;.
\end{aligned}
\tag{4.8}
$$

Here the abbreviations $H'_{0,x}=\partial_x H_0$ and $H''_{0,\xi x}=\partial_\xi\partial_x H_0$, etc. have been employed. These expressions are to be evaluated at $z(t)$. Comparing coefficients of powers of $\hbar$ and of $\big(x-q(t)\big)$ in (4.8) then yields the conditions

$$
\begin{aligned}
\dot\theta&=\dot q p-H_0\;,\\
-\dot p+B\dot q&=H'_{0,x}+BH'_{0,\xi}\;,\\
-\dot B&=H''_{0,xx}+H''_{0,\xi x}B+BH''_{0,\xi x}+BH''_{0,\xi\xi}B\;,\\
\frac{\dot\gamma}{\gamma}&=-\frac{1}{2}\,\mathrm{tr}\big(H''_{0,\xi x}+H''_{0,\xi\xi}B\big)+\mathrm{i}s\dot\varrho\;.
\end{aligned}
\tag{4.9}
$$

With the identification $R_0=\theta$ the first and the second equation immediately imply (4.5) and (4.4), respectively.

The other two equations involve the time evolution $B(t)$ of the complex symmetric $d\times d$ matrix B with positive-definite imaginary part; they determine the action of the metaplectic group on the vector $\varphi^B_{(q,p)}$. At this stage we recall that the symplectic group $\mathrm{Sp}(d,\mathbb{R})$ acts on the Siegel upper half-space (see [Fol89])

$$\Sigma_d:=\{Z\in\mathrm{M}_d(\mathbb{C});\ Z^{\mathrm{T}}=Z,\ \mathrm{Im}\,Z>0\}$$

via

$$S[Z]=(S_{11}Z+S_{12})(S_{21}Z+S_{22})^{-1}\;,\quad\text{where}\quad S=\begin{pmatrix}S_{11}&S_{12}\\S_{21}&S_{22}\end{pmatrix}\in\mathrm{Sp}(d,\mathbb{R})\;.$$

In the present context the differential of the Hamiltonian flow Φ_0^t generated by the classical Hamiltonian H_0 is symplectic, $S_{0,z}(t):=\mathrm{D}\Phi_0^t(z)\in\mathrm{Sp}(d,\mathbb{R})$, and hence can act on the initial value $B\in\Sigma_d$. Indeed,

$$B(t)=S_{0,z}(t)[B]\in\Sigma_d \tag{4.10}$$

yields the solution of the third equation in (4.9) and implies (4.6). The fourth equation requires the introduction of the Maslov multiplier $m(S,Z):=\big(\det(S_{21}Z+S_{22})\big)^{-1/2}$ for $S\in\mathrm{Sp}(d,\mathbb{R})$ and $Z\in\Sigma_d$. This allows us to define the Maslov phase $\sigma(t)$ through

$e^{i\frac{\pi}{2}\sigma(t)} = m(O(t), i\mathbb{1})$, where $O(t)$ is an orthogonal symplectic matrix that is uniquely associated with $S_{0,z}(t)$. One can then show (cf. [Sch01]) that

$$\gamma(t) = \big(\det \operatorname{Im} B(t)\big)^{1/4}\, e^{i\frac{\pi}{2}\sigma(t)+is\varrho(t)} \ .$$

□

We remark that the state (4.3) is closely analogous to the respective solution without spin-orbit coupling. It differs from the latter only by the factor $e^{is\varrho(t)}\phi_{\boldsymbol{n}(t)}$. This observation not only means that quantum mechanically the translational part and the spin part are not entangled, but also on the classical level the translational dynamics are independent of the spin precession $\boldsymbol{n}(t)$. The combination of classical translational and spin motion rather has the structure of a skew product (2.6), indicating that only the spin dynamics depends on the translational part, and not vice versa.

Our aim now is to compare the time evolution generated by the original quantum Hamiltonian $\hat{H}$ with the one generated by the approximate Hamiltonian $\hat{H}_Q(t)$. For this we will follow the method devised in [CR97] for the case without spin. The presence of spin requires some modifications that, however, are modest when the spin quantum number s is fixed. But for the clarity of the presentation, and to prepare for the more involved situation to be dealt with in the second semiclassical scenario, we will now present the argument in some detail.

As stated in section 2 the Hamiltonian $\hat{H}$ generates a unitary and strongly continuous one-parameter group $\hat{U}(t,t_0)$, if its symbol satisfies the ellipticity condition (2.5). When considering the limit $\hbar \to 0$ and keeping s fixed this requirement need only be imposed on the principal symbol, i.e. we demand

$$|H_0(x,\xi) + i| \geq c\,\big(1+|x|^2\big)^{M_x/2}\big(1+|\xi|^2\big)^{M_\xi/2} \ . \tag{4.11}$$

Let now $\hat{U}_Q(t,t_0)$ be the corresponding unitary group generated by $\hat{H}_Q(t)$. Using Duhamel's principle we may then express the difference between these unitary operators as

$$\hat{U}(t,t_0) - \hat{U}_Q(t,t_0) = \frac{1}{i\hbar}\int_{t_0}^{t} \hat{U}(t,t')\big(\hat{H} - \hat{H}_Q(t')\big)\,\hat{U}_Q(t',t_0)\; dt' \ . \tag{4.12}$$

Since we are interested in the difference (3.1), we have to consider the action of (4.12) on the initial state $\varphi^B_{(q,p)} \otimes \phi_{\boldsymbol{n}}$ with $t_0 = 0$. This requires an estimate of

$$\|(\hat{H} - \hat{H}_Q(t'))\psi_Q(t')\| \ , \tag{4.13}$$

where $\psi_Q(t')$ is the time dependent coherent state (4.3). One can achieve this with the help of the following lemma, which is an immediate extension of a result given in [CR97].

Lemma 4.2. *Let $f, g \in C^\infty(T^*\mathbb{R}^d)$ be symbols that satisfy the estimate (2.3) with $M = 0$ and let $F : T^*\mathbb{R}^d \to T^*\mathbb{R}^d$ be a linear map with Hilbert-Schmidt norm $\|F\|_{\mathrm{HS}}$. Fix $\alpha, \beta \in \mathbb{N}^{2d}$ with $k := |\alpha| = |\beta| + 2 > 2$ and introduce the symbol*

$$A(w) := (Fw)^\alpha f(Fw) + \hbar\,(Fw)^\beta g(Fw) \ .$$

Then for any real number $\kappa > 0$ there exist $C > 0$ and $N \in \mathbb{N}$ such that

$$\| \operatorname{op}^W[A]\psi_\hbar\| \leq C\hbar^{k/2} \left(\|F\|_{\mathrm{HS}}^k \sup_{|\gamma|\leq k+N} |\partial_w^\gamma f(w)| + \|F\|_{\mathrm{HS}}^{k-2} \sup_{|\gamma|\leq k-2+N} |\partial_w^\gamma g(w)| \right)$$

holds for any function $\psi_\hbar(x) = \hbar^{-d/4}\psi\big(x/\sqrt{\hbar}\big)$ with $\psi \in \mathscr{S}(\mathbb{R}^d)$ and $0 < \hbar + \sqrt{\hbar}\|F\|_{\mathrm{HS}} < \kappa$.

We intend to apply this lemma to the difference (4.13), with f corresponding to the Taylor remainder of H_0 of order three and g to the Taylor remainder of $\boldsymbol{C} \cdot \mathrm{d}\pi_s(\boldsymbol{\sigma}/2)$ of order one. But first we replace (4.13) by

$$\|\hat{U}_Q(t',0)^*\big(\hat{H} - \hat{H}_Q(t')\big)\hat{U}_Q(t',0)\psi_Q(0)\| \tag{4.14}$$

and invoke an appropriate Egorov theorem. Since the Hamiltonian generating $\hat{U}_Q(t,0)$ has a symbol that is composed of a scalar and quadratic principal part as well as a matrix valued subprincipal part, one can combine the techniques used in [BG00] and [Sch01]. This shows that

$$\hat{W}(t) := \hat{U}_Q(0,t)\big(\hat{H} - \hat{H}_Q(t)\big)\hat{U}_Q(t,0) \tag{4.15}$$

is a Weyl operator with symbol

$$W(t,w) = d^*\big(z(t)\big)\,\big(H - H_Q(t)\big)\big(z - S_{0,z}^{-1}(t)(w - z(t))\big)\,d\big(z(t)\big)\ . \tag{4.16}$$

Here $d\big(z(t)\big)$ is the representation $\pi_s\big(g(t)\big)$ of the solution to equation (3.10) in which $\boldsymbol{C}(t)$ stands for $\boldsymbol{C}\big(z(t)\big)$. Thus

$$d\big(z(t)\big)\phi_{\boldsymbol{n}} = \mathrm{e}^{\mathrm{i}s\varrho(t)}\,\phi_{\boldsymbol{n}(t)}$$

describes the transport of a spin-coherent state along the trajectory $z(t)$. Since the principal part of the symbol $H - H_Q(t)$ is scalar it is not affected by the conjugation with $d\big(z(t)\big)$. In the subprincipal term this conjugation rotates the spin operator $\hat{\boldsymbol{S}} = \hbar\mathrm{d}\pi_s(\boldsymbol{\sigma}/2)$ to $R\big(g(t)\big)\hat{\boldsymbol{S}}$. Therefore, the spin part of the Egorov relation (4.16) does not contribute to an estimate of (4.14) in an essential way.

If one now localises the symbol (4.16) in w with some smooth function that is compactly supported around $z(t)$, leading to an error of size $O(\hbar^\infty)$ when one applies $\hat{W}$ to a coherent state located at $z(t)$, one can proceed to use Lemma 4.2 as in [CR97]. This shows that there exists a constant $K > 0$ such that

$$\|(\hat{H} - \hat{H}_Q(t))\psi_Q(t)\| \leq K\hbar^{3/2}\theta(t)^3\,\delta(t)^m\ , \tag{4.17}$$

where

$$\theta(t) := \max\Big\{1, \sup_{t'\in[0,t]} \|S_{0,z}(t')\|_{\mathrm{HS}}\Big\} \quad \text{and} \quad \delta(t) := \sup_{t'\in[0,t]} \big(1 + |z(t')|\big) \tag{4.18}$$

depend on the classical trajectory $z(t) = (q(t), p(t))$. The constant $m = \max\{M_x, M_\xi\}$ is related to $M = (M_x, M_\xi)$ appearing in (2.3). We then obtain:

Theorem 4.3. *Let the conditions imposed on the Hamiltonian in section 2 and the ellipticity condition (4.11) hold. Then the coherent state $\psi_Q(t)$ defined in (4.3) semiclassically approximates $\psi(t) = \hat{U}(t,0)\big(\varphi^B_{(q,p)} \otimes \phi_{\boldsymbol{n}}\big)$ in the following sense,*

$$\|\psi(t) - \psi_Q(t)\| \leq K\sqrt{\hbar}\, t\, \theta(t)^3 \ . \tag{4.19}$$

The right-hand side vanishes in the combined limits $\hbar \to 0$ and $t \to \infty$ as long as $t \ll T_z(\hbar)$. The time scale $T_z(\hbar)$ depends on the linear stability of the trajectory $z(t)$. If the latter possesses a positive and finite maximal Lyapunov exponent $\lambda_{\max}(z)$, one has $T_z(\hbar) = \frac{1}{6\lambda_{\max}(z)}|\log\hbar|$. In the case of a trajectory on a (non-degenerate) KAM-torus this time scale is $T_z(\hbar) = C\,\hbar^{-1/8}$.

Proof. Conservation of energy, $H_0\big(z(t)\big) = E$, together with the ellipticity condition (4.11) implies that $\delta(t)$ is bounded from above by some constant depending on E. Thus the estimate (4.17) immediately yields (4.19) when used in (4.12).

If $z(t)$ is a trajectory with a positive, but finite, maximal Lyapunov exponent the dominant behaviour as $t \to \infty$ comes from the term $\theta(t)^3$. This is due to the relation

$$\lambda_{\max}(z) = \limsup_{t\to\infty} \frac{1}{t} \log \|S_{0,z}(t)\|_{\mathrm{HS}} \ ,$$

see (A.1), which readily implies $T_z(\hbar) = \frac{1}{6\lambda_{\max}(z)}|\log\hbar|$. In the appendix we also discuss sufficient conditions under which finite maximal Lyapunov exponents occur.

If $z(t)$ is a trajectory on a KAM-torus one can introduce local action-angle variables (I,ϕ) in a neighbourhood of that torus such that in these canonical coordinates the flow reads $I(t) = I$ and $\phi(t) = \phi + \omega(I)t$, see [Laz93]. One therefore finds

$$\|S_{0,z}(t)\|^2_{\mathrm{HS}} = 2d + f(I)\, t^2 \ ,$$

such that $\theta(t) \sim Kt$ as $t \to \infty$, which finally yields $T_z(\hbar) = C\,\hbar^{-1/8}$. In the degenerate case, where $f(I) = 0$, this changes to $T_z(\hbar) = C\,\hbar^{-1/2}$. □

In a next step we want to improve the semiclassical error in (4.19) to an arbitrary (half-integer) power of $\hbar$. This requires higher order approximations that may be achieved as in [CR97] by iterating Duhamel's principle (4.12), resulting in the Dyson expansion

$$\begin{aligned}\hat{U}(t,0) - \hat{U}_Q(t,0) = \sum_{j=1}^{N-1} (\mathrm{i}\hbar)^{-j} \int_0^t \dots \int_{t_{j-1}}^t \hat{U}_Q(t,0)\,\hat{W}(t_j)\dots\hat{W}(t_1)\ \mathrm{d}t_j \dots \mathrm{d}t_1 \\ + R_N(t;\hbar)\end{aligned} \tag{4.20}$$

with remainder term

$$R_N(t;\hbar) = (\mathrm{i}\hbar)^{-N} \int_0^t \dots \int_{t_{N-1}}^t \hat{U}(t,t_N)\,\hat{U}_Q(t_N,0)\,\hat{W}(t_N)\dots\hat{W}(t_1)\ \mathrm{d}t_N \dots \mathrm{d}t_1 \ .$$

In order to estimate the contribution of the remainder when (4.20) is applied to the initial coherent state $\psi(0)=\varphi^B_{(q,p)}\otimes\phi_{\boldsymbol{n}}$ we use the argument leading to (4.17) repeatedly. This yields the bound

$$\|R_N(t;\hbar)\psi(0)\| \leq K_N\, \hbar^{N/2}\, t^N\, \theta(t)^{3N}\, \delta(t)^{mN}\ . \tag{4.21}$$

We then replace the symbol of each difference $\hat{H}-\hat{H}_Q(t_k)$ appearing in the sum in (4.20) by its Taylor expansion,

$$\sum_{|\nu|=3}^{n_k} \frac{1}{\nu!} H_0^{(\nu)}\big(z(t_k)\big)\big(w-z(t_k)\big)^{\nu} + \hbar \sum_{|\nu|=1}^{n_k-2} \frac{1}{\nu!}\big(w-z(t_k)\big)^{\nu} \boldsymbol{C}^{(\nu)}\big(z(t_k)\big)\cdot \mathrm{d}\pi_s(\boldsymbol{\sigma}/2) + r_k(t_k,w)\ . \tag{4.22}$$

The integers n_k are chosen sufficiently large such that, after quantisation, the contribution of the remainder r_k to an application of (4.20) to $\psi(0)$ can be absorbed in the error estimate (4.21). Similar to the case without spin treated in [CR97] the quantisation of the main terms in (4.22) produces matrix valued differential operators $\hat{p}_{kj}(t)=\mathrm{op}^W[p_{kj}(t)]$ with time dependent coefficients acting on the coherent state $\varphi^B_{(q,p)}\otimes\phi_{\boldsymbol{n}}$. The symbols $p_{kj}(t)(x,\xi)$ are polynomials in (x,ξ) of degree $\leq k$. Lemma 4.2 finally leads to the following result:

Theorem 4.4. *Suppose that the quantum Hamiltonian $\hat{H}$ with symbol (2.2) satisfies the conditions specified in section 2 and the ellipticity condition (4.11). Then for $t>0$ and any $N\in\mathbb{N}$ there exists a state $\psi_N(t)\in L^2(\mathbb{R}^d)\otimes\mathbb{C}^{2s+1}$, localised at $\big(q(t),p(t),\boldsymbol{n}(t)\big)$, that approximates the full time evolution $\psi(t)=\hat{U}(t,0)\big(\varphi^B_{(q,p)}\otimes\phi_{\boldsymbol{n}}\big)$ of a coherent state up to an error of order $\hbar^{N/2}$. More precisely,*

$$\|\psi(t)-\psi_N(t)\| \leq C_N \sum_{j=1}^{N-1}\left(\frac{t}{\hbar}\right)^j (\sqrt{\hbar}\theta(t))^{2j+N}\ .$$

The right-hand side vanishes in the combined limits $\hbar\to 0$ and $t\to\infty$ as long as $t\ll T_z(\hbar)$, where $T_z(\hbar)$ denotes the same time scale as in Theorem 4.3.

Furthermore, $\psi_N(t)$ arises from $\varphi^B_{(q,p)}\otimes\phi_{\boldsymbol{n}}$ through the application of certain (time dependent) differential operators $\hat{p}_{kj}(t)=\mathrm{op}^W[p_{kj}(t)]$ of order $\leq k$, followed by the time evolution generated by $\hat{H}_Q(t)$, according to

$$\psi_N(t)=\psi_Q(t)+\sum_{(k,j)\in\Delta_N}\hat{U}_Q(t,0)\,\hat{p}_{kj}(t)\,\psi(0)\ .$$

Here we have defined $\Delta_N:=\{(k,j)\in\mathbb{N}\times\mathbb{N};\ 1\leq k-2j\leq N-1,\ k\geq 3j, 1\leq j\leq N-1\}$.

We remark that the matrix valued differential operators $\hat{p}_{kj}(t)$ do not increase the frequency set of a semiclassical distribution such as the initial state $\varphi^B_{(q,p)}\otimes\phi_{\boldsymbol{n}}$. This follows for the translational part from the respective statement without spin [Rob87], whereas the spin part is only acted upon by a matrix producing linear combinations of $\varphi_{\boldsymbol{n}}$. Moreover, according to Proposition 4.1, $\hat{U}_Q(t,0)$ propagates the frequency set along the trajectory $\big(q(t),p(t),\boldsymbol{n}(t)\big)$ so that both $\psi_Q(t)$ and $\psi_N(t)$ are semiclassically localised at $\big(q(t),p(t),\boldsymbol{n}(t)\big)$.

4.2 Semiclassics with $\hbar s$ fixed

We now consider the second semiclassical scenario in which both semiclassical parameters, $\hbar$ and s, are used. For this purpose we still represent the Hamiltonian $\hat{H}$ as a matrix valued semiclassical Weyl operator. That way $\hbar$ appears as before, whereas the second parameter $s \in \mathbb{N}/2$ controls the dimension of the space $\mathbb{C}^{2s+1}$ on which the symbol operates as a linear map. As we will see, the parameter s enters relevant estimates through the expression $\hbar \mathrm{d}\pi_s(\boldsymbol{\sigma}/2)$. To leading order this will produce factors of $\hbar s$. Our desire to perform systematic semiclassical expansions therefore forces us to keep the combination

$$S := \hbar s$$

fixed in the semiclassical limit. This means that from now on we consider $\hbar \to 0$ and $s \to \infty$ with $\hbar s = S$.

An inspection of Proposition 4.1 and its proof reveals that replacing $\hbar s$ by the constant S will shift the spin-action term $\varrho(t)$, which before was of subleading semiclassical order, to an additional contribution to the action R_0. This suggest that now the translational classical dynamics will be influenced by the spin, requiring a modified quadratic Hamiltonian. Not only that, revisiting the proof of Theorem 4.3 shows that we also have to estimate the application of spin operators to spin-coherent states in terms of s. This requires knowledge of the following:

Lemma 4.5. *For any $X = \boldsymbol{x} \cdot \boldsymbol{\sigma}/2 \in \mathrm{su}(2)$, $\boldsymbol{n} \in \mathrm{S}^2$ and $N \in \mathbb{N}$ there exist differential operators $D_{\boldsymbol{n}}^{(j)}$ of degree $2j$ on $C^\infty(\mathrm{S}^2) \otimes \mathbb{C}^{2s+1}$ and constants $C_N > 0$ such that*

$$\left\| \mathrm{d}\pi_s(X)\phi_{\boldsymbol{n}} - \Big(s + \frac{1}{2}\Big)\Big(1 + \frac{1}{s}\Big) \sum_{j=0}^{N} \frac{1}{s^j} D_{\boldsymbol{n}}^{(j)}\big(\boldsymbol{x} \cdot \boldsymbol{n}\, \phi_{\boldsymbol{n}}\big) \right\| \leq \frac{C_N}{s^{N+1}} \,. \tag{4.23}$$

The leading order in this asymptotic expansion is determined by the constant $D_{\boldsymbol{n}}^{(0)} = 1$,

$$\mathrm{d}\pi_s\big(\boldsymbol{x} \cdot \boldsymbol{\sigma}/2\big)\phi_{\boldsymbol{n}} = s\, \boldsymbol{x} \cdot \boldsymbol{n}\, \phi_{\boldsymbol{n}}\big(1 + O(s^{-1})\big) \,. \tag{4.24}$$

Proof. We start with expressing a linear map L on the representation space $\mathbb{C}^{2s+1}$ in terms of Berezin's quantisation,

$$L = (2s+1) \int_{\mathrm{S}^2} P[L](\boldsymbol{n})\, \Pi(\boldsymbol{n})\; \mathrm{d}\boldsymbol{n} \,, \tag{4.25}$$

where $P[L]$ denotes the upper (or P-) symbol of L, see e.g. [Sim80, Per86]. Furthermore, $\mathrm{d}\boldsymbol{n}$ is the normalised area measure on S^2 and $\Pi(\boldsymbol{n})$ stands for the projector onto the one-dimensional subspace in $\mathbb{C}^{2s+1}$ spanned by the coherent state vector $\phi_{\boldsymbol{n}}$. In the present context the relevant linear maps are representation operators of Lie-algebra elements $X = \boldsymbol{x} \cdot \boldsymbol{\sigma}/2 \in \mathrm{su}(2)$. Their upper symbols are simple,

$$P[\mathrm{d}\pi_s(\boldsymbol{x} \cdot \boldsymbol{\sigma}/2)](\boldsymbol{n}) = (s+1)\, \boldsymbol{x} \cdot \boldsymbol{n} \,,$$

see [Sim80, Per86], so that an application of such an operator to a coherent state reads

$$\mathrm{d}\pi_s(\boldsymbol{x}\cdot\boldsymbol{\sigma}/2)\phi_{\boldsymbol{n}} = (2s+1)(s+1)\int_{\mathrm{S}^2} \boldsymbol{m}\cdot\boldsymbol{x}\,\langle\phi_{\boldsymbol{m}},\phi_{\boldsymbol{n}}\rangle\,\phi_{\boldsymbol{m}}\,\mathrm{d}\boldsymbol{m}\ . \tag{4.26}$$

The coherent states not being defined globally on S^2 is irrelevant to this expression since these states have been defined on a set of full measure.

An asymptotic expansion of the integral (4.26), as $s\to\infty$, can be achieved with the method of steepest descent. This is a variant of the stationary phase method, with a complex phase function, and is described in detail in [Hör90]. The first step consists in identifying the relevant phase factor, which in the present case is given by

$$\langle\phi_{\boldsymbol{n}},\phi_{\boldsymbol{m}}\rangle = \mathrm{e}^{\mathrm{i}s\varphi_{\boldsymbol{n}}(\boldsymbol{m})} \quad \text{with} \quad \operatorname{Im}\varphi_{\boldsymbol{n}}(\boldsymbol{m}) = -\log\left(\frac{1+\boldsymbol{n}\cdot\boldsymbol{m}}{2}\right)\ , \tag{4.27}$$

where $\varphi_{\boldsymbol{n}}$ is independent of s, see [Per86]. Outside of a neighbourhood of $\boldsymbol{m}=-\boldsymbol{n}$ the function $\operatorname{Im}\varphi_{\boldsymbol{n}}$ is finite and non-negative; it has a unique minimum at $\boldsymbol{m}=\boldsymbol{n}$. The real part of the phase $\varphi_{\boldsymbol{n}}$ can be identified as the area of the spherical triangle with edges defined by the north pole, $\boldsymbol{n}$ and $\boldsymbol{m}$. Hence $\boldsymbol{m}=\boldsymbol{n}$ is the unique, non-degenerate stationary point of the phase. Up to an error of size $O(\mathrm{e}^{-s})$ one can hence cut out a neighbourhood of $\boldsymbol{m}=-\boldsymbol{n}$ from the integral (4.26) and use the representation (4.27) for $\operatorname{Im}\varphi_{\boldsymbol{n}}$. The method of steepest descent then implies the existence of differential operators $D^{(j)}_{\boldsymbol{n}}$ of order $2j$ on $C^\infty(\mathrm{S}^2)\otimes\mathbb{C}^{2s+1}$ and constants $C_N>0$ such that for any $N\in\mathbb{N}$ the expansion (4.23) holds. The constant $D^{(0)}_{\boldsymbol{n}}$ fixing the leading order can be identified by choosing $\boldsymbol{x}=\boldsymbol{n}$, since

$$\mathrm{d}\pi_s\big(\boldsymbol{n}\cdot\boldsymbol{\sigma}/2\big)\phi_{\boldsymbol{n}} = s\phi_{\boldsymbol{n}}\ .$$

Comparing with (4.23) therefore yields $D^{(0)}_{\boldsymbol{n}}=1$, which implies (4.24). □

When constructing a quadratic Hamiltonian we now have to take into account that an application of a spin operator to a spin-coherent state contributes to the leading semiclassical order, as (4.24) means

$$\hat{\boldsymbol{S}}\phi_{\boldsymbol{n}} = S\boldsymbol{n}\,\phi_{\boldsymbol{n}} + O(s^{-1})\ .$$

We are therefore led to define a quadratic Hamiltonian $\hat{H}_Q(t)=\mathrm{op}^W[H_Q(t)]$ with matrix valued Weyl symbol as follows,

$$\begin{aligned} H_Q(t,w) = \sum_{|\nu|=0}^{2}\frac{1}{\nu!}H_0^{(\nu)}\big(z(t)\big)\big(w-z(t)\big)^\nu + S\sum_{|\nu|=1}^{2}\frac{1}{\nu!}\boldsymbol{n}(t)\cdot\boldsymbol{C}^{(\nu)}\big(z(t)\big)\big(w-z(t)\big)^\nu \\ + \hbar\boldsymbol{C}\big(z(t)\big)\cdot\mathrm{d}\pi_s(\boldsymbol{\sigma}/2)\ . \end{aligned} \tag{4.28}$$

Like in (4.1) we have introduced a yet to be determined trajectory $z(t)=\big(q(t),p(t)\big)$ in $\mathrm{T}^*\mathbb{R}^d$ with initial condition $z(0)=z=(q,p)$, as well as a curve $\boldsymbol{n}(t)$ on S^2 with $\boldsymbol{n}(0)=\boldsymbol{n}$. This Hamiltonian, being quadratic in $(\hat{Q},\hat{P})$ and linear in $\hat{\boldsymbol{S}}$, propagates an initial coherent state exactly:

Proposition 4.6. *The solution of the quadratic Schrödinger equation*

$$\mathrm{i}\hbar\frac{\partial\psi_Q}{\partial t}(t) = \hat{H}_Q(t)\psi_Q(t) \quad \textit{with} \quad \psi_Q(0) = \varphi^B_{(q,p)} \otimes \phi_{\boldsymbol{n}} \tag{4.29}$$

is, up to an additional phase, again a coherent state,

$$\psi_Q(t) = \mathrm{e}^{\mathrm{i}\left(\frac{R_{\mathrm{so}}(t)}{\hbar}+\frac{\pi}{2}\sigma(t)\right)}\varphi^{B(t)}_{(q(t),p(t))} \otimes \phi_{\boldsymbol{n}(t)} \ . \tag{4.30}$$

Here $\big(q(t), p(t), \boldsymbol{n}(t)\big) = \Phi^t_{\mathrm{so}}(p, q, \boldsymbol{n})$ *is the solution of Hamilton's equations of motion (2.8) on* $\mathrm{T}^*\mathbb{R}^d \times \mathrm{S}^2$ *generated by the classical spin-orbit Hamiltonian*

$$H_{\mathrm{so}}(x, \xi, \boldsymbol{n}) := H_0(x, \xi) + S\boldsymbol{n} \cdot \boldsymbol{C}(x, \xi) \ . \tag{4.31}$$

The phase of $\psi_Q(t)$ *is determined by*

$$R_{\mathrm{so}}(t) = \int_0^t \big(p(t')\dot{q}(t') - H_0(q(t'), p(t'))\big)\,\mathrm{d}t' + S\varrho(t) \ , \tag{4.32}$$

which can be viewed as a total spin-orbit principal function, and by the Maslov phase $\sigma(t)$*. The latter derives from the time evolution*

$$B(t) = \big(\partial_q q(t)B + \partial_p q(t)\big)\big(\partial_q p(t)B + \partial_p p(t)\big)^{-1} \tag{4.33}$$

of the complex symmetric $d \times d$ *matrix* $B \in \Sigma_d$*.*

Proof. The proof of this proposition parallels that of Proposition 4.1; however, a few modifications are necessary. One can again consider (4.30) as an ansatz and determine its ingredients by inserting it into (4.29), leading to equations analogous to (4.8). As opposed to (4.9) the fact that now $S = \hbar s$ is fixed shifts the term with $\varrho(t)$ from the last equation to the first one. Moreover, due to the modified definition of the quadratic Hamiltonian the principal symbol H_0 is replaced by H_{so} in all places but one, yielding

$$\begin{aligned}
\dot{\theta} &= \dot{q}p - H_0 + S\dot{\varrho} \\
-\dot{p} + B\dot{q} &= H'_{\mathrm{so},x} + BH'_{\mathrm{so},\xi} \\
-\dot{B} &= H''_{\mathrm{so},xx} + H''_{\mathrm{so},\xi x}B + BH''_{\mathrm{so},\xi x} + BH''_{\mathrm{so},\xi\xi}B \\
\frac{\dot{\gamma}}{\gamma} &= -\frac{1}{2}\,\mathrm{tr}\big(H''_{\mathrm{so},\xi x} + H''_{\mathrm{so},\xi\xi}B\big) \ .
\end{aligned}$$

The first two equations fix the translational part of the classical dynamics to be solutions of (2.8) with some $\boldsymbol{n}(t)$ and yield the spin-orbit principal function (4.32). In the last two equations H_{so}, which is evaluated at $\big(q(t), p(t), \boldsymbol{n}(t)\big)$, can be viewed as a time dependent Hamiltonian, $\tilde{H}_{\mathrm{so}}(w, t) = H_{\mathrm{so}}(w, \boldsymbol{n}(t))$, for the translational degrees of freedom, with the time dependence introduced through $\boldsymbol{n}(t)$. These equations can be solved in the same manner as in the time independent case, yielding

$$B(t) = S_{\mathrm{so},z}(t)[B]$$

as in (4.10). Here $S_{\mathrm{so},z}(t)$ is a solution of

$$\frac{\mathrm{d}}{\mathrm{d}t} S_{\mathrm{so},z}(t) = J\tilde{H}''_{\mathrm{so}}\big(z(t),t\big)\, S_{\mathrm{so},z}(t) \tag{4.34}$$

with $S_{\mathrm{so},z}(0) = \mathbb{1}_{2d}$; it hence yields (4.33).

The classical spin motion $\boldsymbol{n}(t)$ so far has remained undetermined. Since the equation for the spin-coherent state is again (4.7), it follows that $\boldsymbol{n}(t)$ must be a solution to the spin part of (2.8). □

In contrast to the previous case the classical dynamics that governs the time evolution of the coherent state $\psi_Q(t)$ now is Hamiltonian on the product phase space $\mathrm{T}^*\mathbb{R}^d \times \mathrm{S}^2$, see (2.8). This means that the spin precession is not merely following the translational motion, but there occurs a mutual influence of both dynamics. This effect is caused by the energy scales of the translational and the spin dynamics being comparable in the semiclassical limit, whereas when s is fixed the energy scale of the translational motion dominates.

We now compare the time evolution generated by the full Hamiltonian $\hat{H}$ with the approximate dynamics following from the quadratic Hamiltonian $\hat{H}_Q(t)$ whose symbol is given in (4.28). As opposed to the situation discussed previously, see (4.11), when keeping $\hbar s$ fixed the ellipticity condition has to be imposed on the full symbol of $\hat{H}$, see (2.5), which implies

$$c\,\big(1+|x|^2\big)^{-M_x/2}\big(1+|\xi|^2\big)^{-M_\xi/2} \geq \big\|\big(H(x,\xi)+\mathrm{i}\big)^{-1}\big\| \geq \frac{\big\|\big(H(x,\xi)+\mathrm{i}\big)^{-1}\psi\big\|}{\|\psi\|}\ .$$

Here in the middle $\|\cdot\|$ denotes the operator norm on $\mathbb{C}^{2s+1}$, and on the right-hand side ψ is any non-zero vector in $\mathbb{C}^{2s+1}$. Choosing $\psi = \big(H(x,\xi)+\mathrm{i}\big)^2\phi_{\boldsymbol{n}}$ and using (4.24) we then conclude that the spin-orbit Hamiltonian (4.31) is elliptic, in the sense that

$$|H_{\mathrm{so}}(x,\xi,\boldsymbol{n})+\mathrm{i}| \geq C\,\big(1+|x|^2\big)^{M_x/2}\big(1+|\xi|^2\big)^{M_\xi/2}$$

holds for all $(x,\xi,\boldsymbol{n}) \in \mathrm{T}^*\mathbb{R}^d \times \mathrm{S}^2$. Therefore, we can again base our further investigation of the difference between the two quantum dynamics on the Duhamel relation (4.12). This requires to estimate the analogue of (4.13), where in the present situation $\hat{H} - \hat{H}_Q(t)$ is the Weyl quantisation of the symbol

$$\begin{aligned}\big(H - H_Q(t)\big)(w) = \sum_{|\nu|=1}^{2} \frac{1}{\nu!}\big(\hbar\mathrm{d}\pi_s(\boldsymbol{\sigma}/2) - S\boldsymbol{n}(t)\big)\cdot \boldsymbol{C}^{(\nu)}\big(z(t)\big)\big(w-z(t)\big)^{\nu} \\ + H_0^{[3]}(t,w) + \hbar\boldsymbol{C}^{[3]}(t,w)\cdot \mathrm{d}\pi_s(\boldsymbol{\sigma}/2)\ ,\end{aligned} \tag{4.35}$$

in which $H_0^{[3]}$ and $\boldsymbol{C}^{[3]}$ denote Taylor remainders of order three. Introducing an operator $\hat{W}(t)$ as in (4.15), the same type of an Egorov theorem as above applies, leading to the symbol

$$W(t,w) = d^*\big(z(t)\big)\,\big(H - H_Q(t)\big)\big(z - S_{\mathrm{so},z}^{-1}(t)(w-z(t))\big)\,d\big(z(t)\big) \tag{4.36}$$

of $\hat{W}(t)$. We remark that $z(t)$ being the projection of $\Phi^t_{\rm so}(z,\boldsymbol{n})$ to $\mathrm{T}^*\mathbb{R}^d$ here requires the differential $S_{\mathrm{so},z}(t)$ of $\Phi^t_{\rm so}$ with respect to z. The conjugation with $d\big(z(t)\big)$ has no effect on the scalar terms in (4.35), whereas it rotates the spin operator to $R\big(g(t)\big)\hbar \mathrm{d}\pi_s(\boldsymbol{\sigma}/2)$. Hence, for the application of (4.36) to a spin-coherent state $\phi_{\boldsymbol{n}}$ we can employ Lemma 4.5. By also converting estimates with respect to s into ones with respect to $\hbar$ this yields to leading order

$$\big(R\big(g(t)\big)\hbar \mathrm{d}\pi_s(\boldsymbol{\sigma}/2) - S\boldsymbol{n}(t)\big)\,\phi_{\boldsymbol{n}} = S\,\big(R\big(g(t)\big)\,\boldsymbol{n} - \boldsymbol{n}(t)\big)\phi_{\boldsymbol{n}} + O(s^{-1}) = O(\hbar)\ . \tag{4.37}$$

Moreover, the complete asymptotic series in powers of s^{-1} provided by Lemma 4.5 results in a full asymptotic expansion of (4.37) in powers of $\hbar$. This observation now enables us to apply Lemma 4.2 in a completely analogous way to that used previously, yielding

$$\|(\hat{H} - \hat{H}_Q(t))\psi_Q(t)\| \le K\hbar^{3/2}\theta(t)^3\,\delta(t)^m\ .$$

Here the quantities $\theta(t)$ and $\delta(t)$ are defined as in (4.18), however, now with the differential $S_{\mathrm{so},z}(t)$, and $z(t)$ as given in Proposition 4.6.

The stability of the trajectory $z(t)$ is encoded in the quantity

$$\tilde{\lambda}_{\max}(z) = \limsup_{t\to\infty}\frac{1}{t}\log\|S_{\mathrm{so},z}(t)\|_{\mathrm{HS}}\ . \tag{4.38}$$

Since $z(t)$ is not the integral curve of a flow, rather than calling $\tilde{\lambda}_{\max}(z)$ a Lyapunov exponent we refer to it as a stability exponent. This can, however, be bounded by the maximal Lyapunov exponent of the flow-line $(z(t),\boldsymbol{n}(t))$ in $\mathrm{T}^*\mathbb{R}^d\times\mathrm{S}^2$, see the appendix. Thus, in close analogy to Theorem 4.3 we finally obtain:

Theorem 4.7. *Let the conditions imposed on the Hamiltonian in section 2 hold. Then the coherent state $\psi_Q(t)$ defined in (4.30) semiclassically approximates $\psi(t) = \hat{U}(t,0)\big(\varphi^B_{(q,p)}\otimes\phi_{\boldsymbol{n}}\big)$ in the following sense,*

$$\|\psi(t) - \psi_Q(t)\| \le K\sqrt{\hbar}\,t\,\theta(t)^3\ ,$$

when $\hbar s$ is kept fixed. The right-hand side vanishes in the combined limits $\hbar\to 0$, $s\to\infty$ and $t\to\infty$ as long as $t \ll T_z(\hbar)$. The time scale $T_z(\hbar)$ depends on the linear stability of the trajectory $z(t)$. If the latter possesses a positive and finite stability exponent $\tilde{\lambda}_{\max}(z)$, one has $T_z(\hbar) = \frac{1}{6\tilde{\lambda}_{\max}(z)}|\log\hbar|$. In case $z(t)$ is a projection to $\mathrm{T}^*\mathbb{R}^d$ of a trajectory $(z(t),\boldsymbol{n}(t))$ on a (non-degenerate) KAM-torus in $\mathrm{T}^*\mathbb{R}^d\times\mathrm{S}^2$ this time scale is $T_z(\hbar) = C\,\hbar^{-1/8}$.

As in the previous case an improvement of the semiclassical error can be achieved with the Dyson expansion (4.20). The present case, however, requires an additional estimate of the spin contribution in terms of s. Concerning the error term $R_N(t;\hbar)\psi(0)$, the translational part is dealt with by a repeated application of the argument leading to Theorem 4.7. For the spin part an inspection of the relations (4.35) and (4.36) reveals the necessity to estimate the successive application of the operators

$$\Lambda(t_k) := \boldsymbol{C}^{(\nu)}\big(z(t_k)\big)\cdot\Big(R\big(g(t_k)\big)\hbar\mathrm{d}\pi_s(\boldsymbol{\sigma}/2) - S\boldsymbol{n}(t_k)\Big)$$

to the spin-coherent state $\phi_{\boldsymbol{n}}$. Representing these operators in the form (4.25), the result of their l-fold ($l \leq j$) application reads

$$\begin{aligned}\Lambda(t_l)\ldots\Lambda(t_1)\phi_{\boldsymbol{n}} = (2s+1)^l \int\limits_{\mathrm{S}^2}\ldots\int\limits_{\mathrm{S}^2} P[\Lambda(t_l)](\boldsymbol{m}_l)\ldots P[\Lambda(t_1)](\boldsymbol{m}_1)\times \\ \times\, \Pi(\boldsymbol{m}_l)\ldots\Pi(\boldsymbol{m}_1)\phi_{\boldsymbol{n}}\ \mathrm{d}\boldsymbol{m}_l\ldots\mathrm{d}\boldsymbol{m}_1\ ,\end{aligned} \tag{4.39}$$

with the lower symbols

$$P[\Lambda(t_k)](\boldsymbol{m}_k) = \boldsymbol{C}^{(\nu)}\big(z(t_k)\big)\cdot\Big(S\big(R(g(t_k))\boldsymbol{m}_k - \boldsymbol{n}(t_k)\big) + \hbar R\big(g(t_k)\big)\boldsymbol{m}_k\Big)\ . \tag{4.40}$$

Starting with $\boldsymbol{m}_l$, the integral (4.39) can be successively evaluated with the method of steepest descent similar to the proof of Lemma 4.5. The relation

$$\Pi(\boldsymbol{m}_l)\ldots\Pi(\boldsymbol{m}_1)\phi_{\boldsymbol{n}} = \langle\phi_{\boldsymbol{m}_l},\phi_{\boldsymbol{m}_{l-1}}\rangle\cdots\langle\phi_{\boldsymbol{m}_1},\phi_{\boldsymbol{n}}\rangle\phi_{\boldsymbol{m}_j}$$

then shows that the critical points of the phase are given by $\boldsymbol{m}_l = \boldsymbol{m}_{l-1} = \cdots = \boldsymbol{m}_1 = \boldsymbol{n}$. At these points, however, the lower symbols $P[\Lambda(t_k)](\boldsymbol{m}_k)$ are of order $\hbar$, compare (4.40). The application of the method of steepest descent therefore yields in leading order a contribution $O(\hbar^l) = O(s^{-l})$. Derivatives of total order n contribute terms of the order $O(s^{-n}\hbar^{l-n}) = O(s^{-l})$, if $n \leq l$, and of the order $O(s^{-n})$ otherwise. Altogether there hence exist differential operators $\mathcal{D}^{(\kappa)}$ of order $\leq 2\kappa$ on $C^\infty((\mathrm{S}^2)^l)\otimes\mathbb{C}^{2s+1}$ such that

$$\Lambda(t_l)\ldots\Lambda(t_1)\phi_{\boldsymbol{n}} - \Big(1+\frac{1}{2s}\Big)^l \sum_{\kappa=l}^{K}\frac{1}{s^\kappa}\mathcal{D}^{(\kappa)}\big(P[\Lambda(t_l)](\boldsymbol{m}_l)\ldots P[\Lambda(t_1)](\boldsymbol{m}_1)\phi_{\boldsymbol{n}}\big)_{\boldsymbol{m}_l=\cdots=\boldsymbol{m}_1=\boldsymbol{n}} \tag{4.41}$$

is of the order $s^{-(K+1)}$ for any $K \geq l$. The left-hand side of (4.39) hence is of the order $O(s^{-l}) = O(\hbar^l)$, meaning that every factor $\Lambda(t_k)$ contributes a factor of $\hbar$. We therefore finally obtain an estimate of the remainder term to the Dyson series given by

$$\|R_N(t;\hbar)\psi(0)\| \leq K_N\hbar^{N/2}t^N\theta(t)^{3N}\delta(t)^{mN}\ .$$

The main terms in the Dyson expansion are treated by replacing each factor of (4.35), occurring at $t = t_k$, with the Taylor expansions

$$\begin{aligned}&\sum_{|\nu|=1}^{2}\frac{1}{\nu!}\big(\hbar\mathrm{d}\pi_s(\boldsymbol{\sigma}/2) - S\boldsymbol{n}(t_k)\big)\cdot\boldsymbol{C}^{(\nu)}\big(z(t_k)\big)\big(w - z(t_k)\big)^\nu \\ &\qquad + \sum_{\nu=3}^{n_k}\frac{1}{\nu!}\Big(H_0^{(\nu)}\big(z(t_k)\big) + \hbar\boldsymbol{C}^{(\nu)}\big(z(t_k)\big)\mathrm{d}\pi_s(\boldsymbol{\sigma}/2)\Big)\big(w - z(t_k)\big)^\nu + r_k(t_k,w)\ ,\end{aligned}$$

where again the integers n_k are chosen sufficiently large. The contribution of the translational degrees of freedom can be dealt with as in the previous semiclassical scenario, and the spin contribution follows from the expansion (4.41). Finally grouping together terms of corresponding orders in $\hbar$, we arrive at a statement analogous to Theorem 4.4.

Theorem 4.8. *Suppose that the quantum Hamiltonian $\hat{H}$ with symbol (2.2) satisfies the conditions specified in section 2. Then for $t > 0$ and any $N \in \mathbb{N}$ there exists a state $\psi_N(t) \in L^2(\mathbb{R}^d) \otimes \mathbb{C}^{2s+1}$, localised at $\big(q(t), p(t), \boldsymbol{n}(t)\big)$, that approximates the full time evolution $\psi(t) = \hat{U}(t,0)\big(\varphi^B_{(q,p)} \otimes \phi_{\boldsymbol{n}}\big)$ of a coherent state up to an error of order $\hbar^{N/2}$ when $\hbar s$ is fixed. More precisely,*

$$\|\psi(t) - \psi_N(t)\| \leq C_N \sum_{j=1}^{N-1} \left(\frac{t}{\hbar}\right)^j (\sqrt{\hbar}\theta(t))^{2j+N} \ .$$

The right-hand side vanishes in the combined limits $\hbar \to 0$, $s \to \infty$ and $t \to \infty$ as long as $t \ll T_z(\hbar)$, where $T_z(\hbar)$ denotes the same time scale as in Theorem 4.7.

Furthermore, $\psi_N(t)$ arises from $\varphi^B_{(q,p)} \otimes \phi_{\boldsymbol{n}}$ through the application of certain (time dependent) differential operators $\hat{q}_{k\kappa j}(t) = \mathrm{op}^W[p_{kj}(t)] \otimes r_\kappa$,

$$\psi_N(t) = \psi_Q(t) + \sum_{(k,\kappa,j)\in\Delta_N} \hat{U}_Q(t,0)\, \hat{q}_{k\kappa j}(t)\, \psi(0) \ ,$$

where $p_{kj}(t)$ is a polynomial in (x,ξ) of degree $\leq k$ and r_κ is a differential operator of order $\leq 2\kappa$ on $C^\infty(\mathrm{S}^2) \otimes \mathbb{C}^{2s+1}$. Here we have also defined

$$\Delta_N := \{(k,\kappa,j) \in \mathbb{N}^3;\ 1 \leq k + 2\kappa - 2j \leq N-1,\ k + 2\kappa \geq 3j,\ 1 \leq j \leq N-1\} \ .$$

The semiclassical localisation of $\psi_N(t)$ here is different from the situation covered by Theorem 4.4 in that the operators r_κ act on $\phi_{\boldsymbol{n}}$. But these are differential operators and hence do not increase the frequency set. This means that $\psi_N(t)$ is semiclassically localised at $\Phi^t_{\mathrm{so}}(q,p,\boldsymbol{n})$ and in in this respect is not different from the classically propagated coherent state $\psi_Q(t)$.

5 Discussion

In the previous section we analysed the semiclassical behaviour of coherent states in two different limits. In various places we saw that the difference between the two cases is expressed in the way the classical translational and spin motion are coupled. Otherwise the final results agree to a large extent. This includes the mechanisms of semiclassical localisation in the product phase space $\mathrm{T}^*\mathbb{R}^d \times \mathrm{S}^2$.

The problem of how the localisation of an initial coherent state develops with time can be made more explicit by using semiclassical phase-space lifts of the coherent states. At $t = 0$ the state $\psi(0) = \varphi^B_{(q,p)} \otimes \phi_{\boldsymbol{n}}$ is concentrated in a neighbourhood of the point $(q,p,\boldsymbol{n}) \in \mathrm{T}^*\mathbb{R}^d \times \mathrm{S}^2$. This concentration can be measured in terms of expectation values $\langle \psi(0), \hat{A}\psi(0)\rangle$ of operators $\hat{A} = \mathrm{op}^W[A]$ that are quantisations of well localised symbols $A \in C_0^\infty(\mathrm{T}^*\mathbb{R}^d) \otimes \mathrm{M}_{2s+1}(\mathbb{C})$. For simplicity we also assume that A is independent of $\hbar$. At later times $\psi(t)$ can in both semiclassical scenarios be approximated by an appropriate coherent state $\psi_Q(t)$, such that

$$\langle \psi(t), \hat{A}\psi(t)\rangle = \langle \psi_Q(t), \hat{A}\psi_Q(t)\rangle + o(1) \ , \quad t \ll T_z(\hbar) \ . \tag{5.1}$$

The expectation value on the right-hand side has a phase-space representation

$$\langle\psi_Q(t),\hat{A}\psi_Q(t)\rangle = \frac{1}{(2\pi\hbar)^d}\iint_{\mathrm{T}^*\mathbb{R}^d} W[\varphi_{z(t)}^{B(t)}](w)\,\langle\phi_{\boldsymbol{n}(t)},A(w)\phi_{\boldsymbol{n}(t)}\rangle_{\mathbb{C}^{2s+1}}\,\mathrm{d}w\;. \tag{5.2}$$

A comparison with (3.5) clearly reveals that the state $\psi_Q(t)$ is concentrated at the point $(q(t),p(t),\boldsymbol{n}(t))$ in the semiclassical limit as long as the quadratic form $G_{B(t)}/\hbar$ is strictly positive definite. Either of the time evolutions (4.6) and (4.33) of B now imply [Sch01]

$$G_{B(t)} = (S_z(t)^{-1})^*\,G_B\,S_z(t)^{-1}\;,$$

so that the spreading of $\psi_Q(t)$ in $\mathrm{T}^*\mathbb{R}^d$, see (3.6), is bounded according to

$$\frac{\hbar}{\operatorname{tr}G_{B(t)}} \le \frac{\hbar}{\|G_{B(t)}\|_{\mathrm{HS}}} \le \frac{\hbar\|S_z(t)\|_{\mathrm{HS}}^2}{\|G_B\|_{\mathrm{HS}}}\;.$$

Here $S_z(t)$ denotes the differential of the appropriate flow with respect to (x,ξ). If $z(t)$ now is a trajectory with maximal Lyapunov (or stability) exponent $\lambda_{\max}(z)>0$, the requirement for the state $\psi_Q(t)$ to remain localised therefore is $t\ll\frac{1}{2\lambda_{\max}(z)}|\log\hbar|$. This time scale is three times larger than $T_z(\hbar)$, which is the estimated time in (5.1) for the coherent state $\psi_Q(t)$ to still well approximate the full time evolution $\psi(t)$.

Let us remark that the limitations in (5.1), to approximate the expectation value in terms of a coherent state, derive from estimating the difference $\psi(t)-\psi_Q(t)$ in L^2-norm. But the error term on the right-hand side of (5.1) measures this difference in a considerably weaker form so that one might expect it to vanish as $\hbar\to 0$ and $t\to\infty$ also for times $T_z(\hbar)\le t\ll 3T_z(\hbar)$. In the case without spin Bouzouina and Robert [BR02] proved that this indeed holds, suggesting that the same is true in the present setting.

Expectation values in coherent states such as (5.1) can also be used to obtain the leading semiclassical description of the propagation of observables. To see this let $\hat{A}$, as above, be a bounded Weyl operator and denote its quantum time evolution by $\hat{A}(t)=\hat{U}(t,0)^*\hat{A}\,\hat{U}(t,0)$. Here, however, we do not necessarily require the symbol to be compactly supported. The relations (5.1) and (5.2) then remain valid so that

$$\langle\psi(0),\hat{A}(t)\psi(0)\rangle = \frac{1}{(2\pi\hbar)^d}\iint_{\mathrm{T}^*\mathbb{R}^d} W[\varphi_{z(t)}^{B(t)}](w)\,\langle\phi_{\boldsymbol{n}(t)},A(w)\phi_{\boldsymbol{n}(t)}\rangle_{\mathbb{C}^{2s+1}}\,\mathrm{d}w + o(1)\;.$$

Since $\hat{A}(t)$ is bounded it may also be expressed as a Weyl operator, with symbol $A(t)$ such that for $t\ll T_z(\hbar)$ equation (5.1) can be rewritten as

$$\begin{aligned}\frac{1}{(2\pi\hbar)^d}&\iint_{\mathrm{T}^*\mathbb{R}^d} W[\varphi_{z(0)}^{B(0)}](w)\,\langle\phi_{\boldsymbol{n}(0)},A(t)(w)\phi_{\boldsymbol{n}(0)}\rangle_{\mathbb{C}^{2s+1}}\,\mathrm{d}w\\ &-\frac{1}{(2\pi\hbar)^d}\iint_{\mathrm{T}^*\mathbb{R}^d} W[\varphi_{z(t)}^{B(t)}](w)\,\langle\phi_{\boldsymbol{n}(t)},A(w)\phi_{\boldsymbol{n}(t)}\rangle_{\mathbb{C}^{2s+1}}\,\mathrm{d}w = o(1)\;.\end{aligned}$$

The semiclassical localisation properties of the coherent states discussed above therefore imply that in leading order the symbol of the time evolved observable $\hat{A}(t)$ can be expressed in terms of the symbol of $\hat{A}$ transported along the classical flow $\big(q(t),p(t),\boldsymbol{n}(t)\big)$,

$$\langle\phi_{\boldsymbol{n}},A(t)(q,p)\phi_{\boldsymbol{n}}\rangle_{\mathbb{C}^{2s+1}} - \langle\phi_{\boldsymbol{n}(t)},A\big(q(t),p(t)\big)\phi_{\boldsymbol{n}(t)}\rangle_{\mathbb{C}^{2s+1}} = o(1)\;.$$

The $\mathbb{C}^{2s+1}$-expectation values in spin-coherent states are lower (or Q-) symbols (see e.g. [Sim80, Per86]) of the matrix valued functions $A(t)$ and A, respectively. In terms of this mixed phase space representation of operators, employing Weyl calculus for the translational part and Q-symbols for the spin part, this means that the quantum time evolution of observables follows the classical dynamics in leading semiclassical order. This statement represents a limited version of an Egorov theorem and again is valid for both semiclassical scenarios discussed in the preceding section, up to the time scale $t \ll T_z(\hbar)$.

Acknowledgments

A major part of this work has been performed when both authors stayed at the Mathematical Sciences Research Institute, Berkeley. We would like to thank the MSRI for its hospitality and for the support extended to us. Financial support by the Deutsche Forschungsgemeinschaft under contract no. Ste 241/15-2 is gratefully acknowledged. R.G. was also supported through the Doktorandenstipendium D/02/47460 by Deutscher Akademischer Austauschdienst.

Appendix: Linear stability of Hamiltonian flows

The flows Φ_0^t and Φ_{so}^t introduced in section 2 are both Hamiltonian flows on symplectic phase spaces. They are generated by smooth Hamiltonian functions H on $2n$-dimensional smooth manifolds M with symplectic forms ω. In the first case the Hamiltonian is $H_0(x,\xi)$, defined on the phase space $M = \mathrm{T}^*\mathbb{R}^d$ so that $n = d$ and $\omega = \mathrm{d}x \wedge \mathrm{d}\xi$. In the situation of classical spin-orbit coupling the Hamiltonian $H_{\mathrm{so}}(x,\xi,\boldsymbol{n})$ is given on $M = \mathrm{T}^*\mathbb{R}^d \times \mathrm{S}^2$. Thus, $n = d+1$ and $\omega = \mathrm{d}x \wedge \mathrm{d}\xi + \mathrm{d}\boldsymbol{n}$, where $\mathrm{d}\boldsymbol{n}$ denotes the normalised area two-form on the sphere S^2. In this appendix we want to recall the notion of Lyapunov exponents and give sufficient criteria of their existence in terms of properties of the Hamiltonian function.

The linear stability of a flow Φ^t is determined by properties of the differential $\mathrm{D}\Phi^t(\alpha)$ which is a linear map from the tangent space $\mathrm{T}_\alpha M$ to $\mathrm{T}_{\Phi^t(\alpha)}M$. It, moreover, is a multiplicative cocycle over the flow Φ^t, i.e. $\mathrm{D}\Phi^{t+t'}(\alpha) = \mathrm{D}\Phi^{t'}(\Phi^t(\alpha))\,\mathrm{D}\Phi^t(\alpha)$. If one introduces a euclidean scalar product in the tangent spaces, this gives rise to the adjoint $\mathrm{D}\Phi^t(\alpha)^*$. Then $\mathrm{D}\Phi^t(\alpha)^*\,\mathrm{D}\Phi^t(\alpha)$ is a non-negative symmetric linear map on $\mathrm{T}_\alpha M$ whose eigenvalues we denote by

$$\mu_t^{(1)}(\alpha) \geq \cdots \geq \mu_t^{(2n)}(\alpha) \geq 0 \ .$$

The $2n$ Lyapunov exponents of the flow Φ^t at $\alpha \in M$ are now given by the expressions

$$\lambda_k(z) := \limsup_{t\to\infty} \frac{1}{2t} \log \mu_t^{(k)}(z) \ ,$$

if these are finite. The largest Lyapunov exponent $\lambda_{\max}(\alpha)$ provides a quantitative measure for the linear stability of Φ^t since it measures the leading rate of local phase space expansion;

it can be obtained from the relation

$$\lambda_{\max}(\alpha) = \limsup_{t\to\infty} \frac{1}{2t} \log \operatorname{tr}\bigl(\mathrm{D}\Phi^t(\alpha)^* \, \mathrm{D}\Phi^t(\alpha)\bigr) \ . \tag{A.1}$$

Hamiltonian flows leave the energy shells

$$\Omega_E := \{\alpha \in M;\ H(\alpha) = E\}$$

invariant. If E is a regular value of the Hamiltonian function H, the energy shell Ω_E is a smooth submanifold of M of dimension $2n-1$. In such a case two Lyapunov exponents are always zero. They correspond to the direction of the flow and the direction transversal to the energy shell. Of the remaining $2n-2$ Lyapunov exponents half are non-negative (if they exist) and the rest of the Lyapunov spectrum is given by minus the first half.

In general it is not known whether the Lyapunov exponents are finite. If, however, an energy shell Ω_E is compact, one can introduce the normalised Liouville measure as a flow invariant probability measure on Ω_E. In this case one can apply Oseledec' multiplicative ergodic theorem to the restriction of Φ^t to this energy shell [Ose68]; it guarantees that the Lyapunov exponents are finite for almost all points on Ω_E with respect to Liouville measure. Moreover, if the flow is ergodic with respect to Liouville measure $\lambda_k(\alpha)$ is constant on a set of full measure. Since we want to consider also non-compact energy shells we now give alternative sufficient criteria for the finiteness of Lyapunov spectra.

Proposition A.1. *Let $H \in C^\infty(M)$ be a Hamiltonian function such that the Hilbert-Schmidt norm of D^2H is bounded on the energy shell $\Omega_{E,\alpha}$ that contains the point $\alpha \in M$. Then the Lyapunov exponents $\lambda_1(\alpha), \ldots, \lambda_{2n}(\alpha)$ are finite.*

Proof. Fix $\alpha \in M$ and introduce canonical coordinates $(q,p) \in U \subset \mathbb{R}^n \times \mathbb{R}^n$ in a neighbourhood of α. Then in this neighbourhood D^2H is represented by the matrix $H''(q,p)$ of second derivatives with respect to (q,p). In these coordinates we denote the flow by $\tilde{\Phi}^t(q,p)$; its differential satisfies the equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{D}\tilde{\Phi}^t(q,p) = J\, H''\bigl(\tilde{\Phi}^t(q,p)\bigr)\, \mathrm{D}\tilde{\Phi}^t(q,p) \ , \qquad \mathrm{D}\tilde{\Phi}^t(q,p)|_{t=0} = \mathbb{1}_{2n} \ , \tag{A.2}$$

where $J = \left(\begin{smallmatrix} 0 & \mathbb{1}_n \\ -\mathbb{1}_n & 0 \end{smallmatrix}\right)$. By integrating (A.2) and taking the Hilbert-Schmidt norm one obtains

$$\|\mathrm{D}\tilde{\Phi}^t(q,p)\|_{\mathrm{HS}} \le 2n + \int_0^t \|J\, H''\bigl(\tilde{\Phi}^s(q,p)\bigr)\|_{\mathrm{HS}}\, \|\mathrm{D}\tilde{\Phi}^s(q,p)\|_{\mathrm{HS}}\ \mathrm{d}s \ .$$

For simplicity we here assume that for the points $\Phi^s(\alpha)$, $s \in [0,t]$, one can use the same system of canonical coordinates. Gronwall's inequality then yields the estimate ($t > 0$)

$$\|\mathrm{D}\tilde{\Phi}^t(q,p)\|_{\mathrm{HS}} \le 2n \exp\Bigl\{t \sup_{s\in[0,t]} \|J\, H''\bigl(\tilde{\Phi}^s(q,p)\bigr)\|_{\mathrm{HS}}\Bigr\} \le 2n\, \mathrm{e}^{Ct} \ ,$$

with some constant $C > 0$. The last line follows from the boundedness of $\mathrm{D}^2 H$ on $\Omega_{E,\alpha}$. Since on the other hand

$$\|\mathrm{D}\tilde{\Phi}^t(q,p)\|_{\mathrm{HS}} = \sqrt{\mu_t^{(1)}(\alpha) + \cdots + \mu_t^{(2n)}(\alpha)}\ ,$$

the bound

$$\frac{1}{2t} \log \mu_t^{\max}(\alpha) \leq K$$

for the maximal eigenvalue $\mu_t^{\max}(\alpha)$ follows. This finally implies the assertion. $\square$

An application of this Proposition to the two flows Φ_0^t (defined on $M = \mathrm{T}^*\mathbb{R}^d$) and Φ_{so}^t (defined on $M = \mathrm{T}^*\mathbb{R}^d \times \mathrm{S}^2$) immediately yields

Corollary A.2. *If the norm of H_0'' is bounded on $\Omega_{E,(x,\xi)} \subset \mathrm{T}^*\mathbb{R}^d$, the $2d$ Lyapunov exponents $\lambda_{0,k}(x,\xi)$ of the flow Φ_0^t are finite. If, in addition, the derivatives $\boldsymbol{C}^{(\nu)}(x',\xi')$ of order $|\nu| \leq 2$ are bounded for all $(x',\xi',\boldsymbol{n}') \in \Omega_{E,(x,\xi,\boldsymbol{n})} \subset \mathrm{T}^*\mathbb{R}^d \times \mathrm{S}^2$, the $2d+2$ Lyapunov exponents $\lambda_{\mathrm{so},k}(x,\xi,\boldsymbol{n})$ of the flow Φ_{so}^t are also finite.*

In the second semiclassical scenario, however, rather than the Lyapunov exponent $\lambda_{\mathrm{so},k}(q,p,\boldsymbol{n})$ of a point $(q,p,\boldsymbol{n}) \in \mathrm{T}^*\mathbb{R}^d \times \mathrm{S}^2$ the stability exponent (4.38) of the projection to $\mathrm{T}^*\mathbb{R}^d$ entered Theorem 4.7. Revisiting the proof of Proposition A.1 shows that in view of (4.34) such a stability exponent is finite under the same conditions as stated in Corollary A.2 for $\lambda_{\mathrm{so},k}$. Moreover, a simple estimate yields the bound

$$\tilde{\lambda}_{\max} \leq \lambda_{\mathrm{so},\max}\ .$$

References

[BB00] F. Bonechi and S. De Bièvre, *Exponential mixing and $|\ln \hbar|$ time scales in quantized hyperbolic maps on the torus*, Commun. Math. Phys. **211** (2000), 659–686.

[BG00] J. Bolte and R. Glaser, *Quantum ergodicity for Pauli Hamiltonians with spin* 1/2, Nonlinearity **13** (2000), 1987–2003.

[BG04] J. Bolte and R. Glaser, *A semiclassical Egorov theorem and quantum ergodicity for matrix valued operators*, Commun. Math. Phys., to appear, arXiv math-ph/0204018, 2004.

[BGK01] J. Bolte, R. Glaser, and S. Keppeler, *Quantum and classical ergodicity of spinning particles*, Ann. Phys. (NY) **293** (2001), 1–14.

[BK99a] J. Bolte and S. Keppeler, *A semiclassical approach to the Dirac equation*, Ann. Phys. (NY) **274** (1999), 125–162.

[BK99b] J. Bolte and S. Keppeler, *Semiclassical form factor for chaotic systems with spin* 1/2, J. Phys. A: Math. Gen. **32** (1999), 8863–8880.

[BM69] A. Bohr and B. R. Mottelson, *Nuclear Structure*, vol. 1, Benjamin, Reading, Mass., 1969.

[BR02] A. Bouzouina and D. Robert, *Uniform semiclassical estimates for the propagation of quantum observables*, Duke Math. J. **111** (2002), 223–252.

[CFS82] I. P. Cornfeld, S. V. Fomin, and Ya. G. Sinai, *Ergodic Theory*, Grundlehren der mathematischen Wissenschaften, vol. 245, Springer-Verlag, Berlin, Heidelberg, New York, 1982.

[Chi79] B. V. Chirikov, *A universal instability of many-dimensional oscillator systems*, Phys. Rep. **52** (1979), 264–379.

[CR97] M. Combescure and D. Robert, *Semiclassical spreading of quantum wave packets and applications near unstable fixed points of the classical flow*, Asymptot. Anal. **14** (1997), 377–404.

[DS99] M. Dimassi and J. Sjöstrand, *Spectral Asymptotics in the Semi-Classical Limit*, London Mathematical Society Lecture Notes, vol. 268, Cambridge University Press, Cambridge, 1999.

[Fol89] G. B. Folland, *Harmonic Analysis in Phase Space*, Annals of Mathematics Studies, vol. 122, Princeton University Press, Princeton, New Jersey, 1989.

[Hel75] E. J. Heller, *Time-dependent approach to semiclassical dynamics*, J. Chem. Phys. **62** (1975), 1544–1555.

[HJ00] G. A. Hagedorn and A. Joye, *Exponentially accurate semiclassical dynamics: propagation, localization, Ehrenfest times, scattering, and more general states*, Ann. Henri Poincaré **1** (2000), 837–883.

[Hör90] L. Hörmander, *The Analysis of Linear Partial Differential Operators I*, 2nd ed., Grundlehren der mathematischen Wissenschaften, vol. 256, Springer-Verlag, Berlin, Heidelberg, New York, 1990.

[HPS83] H. Hogreve, J. Potthoff, and R. Schrader, *Classical limits for quantum particles in external Yang-Mills potentials*, Commun. Math. Phys. **91** (1983), 573–598.

[Kep03] S. Keppeler, *Semiclassical quantisation rules for the Dirac and Pauli equations*, Ann. Phys. (NY) **304** (2003), 40–71.

[KS85] J. R. Klauder and B. S. Skagerstam (eds.), *Coherent States. Applications in Physics and Mathematical Physics*, World Scientific, Singapore, 1985.

[KW02] S. Keppeler and R. Winkler, *Anomalous magneto-oscillations and spin precession*, Phys. Rev. Lett. **88** (2002), 046401.

[Laz93] V. F. Lazutkin, *KAM Theory and Semiclassical Approximation to Eigenfunctions*, Ergebnisse der Mathematik und ihrer Grenzgebiete, vol. 24, Springer-Verlag, Berlin, Heidelberg, New York, 1993.

[Lit86] R. G. Littlejohn, *The semiclassical evolution of wave packets*, Phys. Rep. **138** (1986), 193–291.

[Ose68] V. I. Oseledec, *A multiplicative ergodic theorem. Lyapunov characteristic numbers for dynamical systems*, Trans. Moscow Math. Soc. **19** (1968), 197–231.

[Per86] A. Perelomov, *Generalized Coherent States and Their Applications*, Texts and Monographs in Physics, Springer-Verlag, Berlin, Heidelberg, New York, 1986.

[Rob87] D. Robert, *Autour de l'Approximation Semi-Classique*, Progress in Mathematics, vol. 68, Birkhäuser, Boston, Basel, Stuttgart, 1987.

[SB02] P. G. Silvestrov and C. P. J. Beenakker, *Ehrenfest times for classically chaotic systems*, Phys. Rev. E. **65** (2002), 035208(R).

[Sch26] E. Schrödinger, *Der stetige Übergang von der Mikro- zur Makromechanik*, Naturwissenschaften **14** (1926), 664–666.

[Sch01] R. Schubert, *Semiclassical localization in phase space*, Ph.D. thesis, Universität Ulm, 2001.

[Sch04] R. Schubert, *Semiclassical behaviour of expectation values in time evolved Lagrangian states for large times*, preprint, 2004, available at arXiv:math.MP/0402038.

[SFHŽ01] S. Das Sarma, J. Fabiana, X. Hua, and I. Žutić, *Spin electronics and spin computation*, Solid State Commun. **119** (2001), 207–215.

[Sim80] B. Simon, *The classical limit of quantum partition functions*, Commun. Math. Phys. **71** (1980), 247–276.

[Zas81] G. M. Zaslavsky, *Stochasticity in quantum systems*, Phys. Rep. **80** (1981), 157–250.