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Zitterbewegung and semiclassical observables for the Dirac equation

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Abstract

In a semiclassical context we investigate the Zitterbewegung of relativistic particles with spin $1/2$ moving in external fields. It is shown that the analogue of Zitterbewegung for general observables can be removed to arbitrary order in $\hbar$ by projecting to dynamically almost invariant subspaces of the quantum mechanical Hilbert space which are associated with particles and anti-particles. This not only allows us to identify observables with a semiclassical meaning, but also to recover combined classical dynamics for the translational and spin degrees of freedom. Finally, we discuss properties of eigenspinors of a Dirac–Hamiltonian when these are projected to the almost invariant subspaces, including the phenomenon of quantum ergodicity.

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1. Introduction

When Dirac had introduced his relativistic quantum theory for spin-$1/2$ particles it soon became clear that despite its overwhelming success in producing the correct hydrogen spectrum, including fine structure, this theory was plagued with a number of apparent inconsistencies as, e.g., Klein's paradox [Kle29]. Schrödinger observed [Sch30] that the (free) time evolution of the naive position operator, which he had taken over from non-relativistic quantum mechanics, contained a contribution without any classical interpretation. Since this term was rapidly oscillating he introduced the notion of *Zitterbewegung (trembling motion)*. Schrödinger wanted to explain this effect as being caused by spin. Later, however, it became clear that all paradoxes stemmed from the coexistence of particles and anti-particles in Dirac's theory, and that only a quantum field theoretic description, predicting pair creation and annihilation, could cure these problems in a fully satisfactory manner.

It nevertheless turned out that relativistic quantum mechanics was capable of describing many important physical phenomena; e.g., in atomic physics it serves to explain spectra of large atoms and in nuclear physics it allows us to construct models of nuclei. Within the context of this theory one can remove the Zitterbewegung of free particles by introducing modified position operators that are associated with either only particles or only anti-particles. These operators are free from the particle/anti-particle interferences that cause the Zitterbewegung; for details see, e.g., [Tha92]. In the case of interactions (with external potentials) the Zitterbewegung cannot be exactly eliminated. It is, however, possible to devise an asymptotic construction, e.g. based on the Foldy–Wouthuysen transformation. This involves a non-relativistic expansion, and when applied to the Dirac equation, reproduces in leading order the Pauli equation. The genuinely relativistic coexistence of particles and anti-particles is therefore removed in a natural way.

Similar constructions are possible in a semiclassical context while maintaining the relativistic level of description. The decoupling of particles from anti-particles then proceeds asymptotically order by order in powers of the semiclassical parameter $\hbar$. In this direction several approaches have been developed recently, aiming at semiclassical expansions for scattering phases [BN99, BR99] or at recovering the Thomas precession of the spin [Spo00], see also [Cor01, Teu03]. In other semiclassical approaches trace formulae of the Gutzwiller type have been derived [BK98, BK99], see also [Kep03]. Here our goal is to introduce a general semiclassical framework for the Dirac equation, and in particular to identify a sufficiently large algebra of quantum mechanical observables that can be assigned a classical analogue in a way that is consistent with the dynamics. And in contrast to previous studies we do not construct semiclassical (unitary) Foldy–Wouthuysen operators but use the associated projection operators, thus avoiding ambiguities in the choice of the unitaries.

The outline of this paper is as follows. In section 2 we recall the phenomenon of Zitterbewegung of free relativistic particles, emphasizing that this effect can be removed through an introduction of suitably modified position operators. The following section is devoted to the construction of projection operators that semiclassically separate particles from anti-particles in the presence of an interaction with external potentials. Quantum observables with a semiclassical meaning are introduced in section 4, and a characterization of such observables that maintain this property under their time evolution is provided. Section 5 contains a discussion of the classical dynamics emerging from the quantum dynamics generated by a Dirac–Hamiltonian in the semiclassical limit. It is shown that a combined time evolution of the translational and the spin degrees of freedom arises in the form of a so-called skew-product. Finally, in section 6 we discuss to what extent eigenspinors of a Dirac–Hamiltonian can be associated with either particles or anti-particles. We also show that an ergodic behaviour of the combined classical dynamics implies quantum ergodicity, i.e. a semiclassical equidistribution on particle and anti-particle energy shells of eigenspinor projections to the respective energy shells.

2. Zitterbewegung for the free motion

Since its early discovery by Schrödinger Zitterbewegung has mostly been discussed in the context of the Dirac equation for a free relativistic particle of mass m and spin $1/2$, whose Hamiltonian reads

$$\hat{H}_0 := -\mathrm{i}\hbar c\boldsymbol{\alpha}\cdot\nabla + \beta mc^2. \tag{2.1}$$

The relations $\alpha_k\alpha_l + \alpha_l\alpha_k = 2\delta_{kl}$ and $\alpha_k\beta + \beta\alpha_k = 0$ $(k, l = 1, 2, 3)$ defining the Dirac algebra are realized by the 4×4 matrices

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} \qquad \text{and} \qquad \beta = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}$$

where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the vector of Pauli spin matrices and $\mathbb{1}_n$ denotes the $n \times n$ unit matrix. The operator (2.1) is essentially self-adjoint on the dense domain $C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^4$ in the Hilbert space $\mathscr{H} := L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$; its spectrum is absolutely continuous and comprises $(-\infty, -mc^2) \cup (mc^2, \infty)$; see e.g., [Tha92]. The time evolution (free motion)

$$\hat{U}_0(t) := \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0 t}$$

hence is unitary.

In his seminal paper [Sch30] Schrödinger solved the free time evolution of the standard position operator $\hat{\boldsymbol{x}}$, whose components are defined as multiplication operators on a suitable domain in $L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$. His intention was to resolve the apparent paradox that the spectrum of the velocity operator resulting from the Heisenberg equation of motion for the standard position operator, $\dot{\hat{\boldsymbol{x}}}(t) = c\boldsymbol{\alpha}(t)$, consists of $\pm c$, whereas the classical velocity of a free relativistic particle reads $c^2\boldsymbol{p}/\sqrt{\boldsymbol{p}^2c^2 + m^2c^4}$ and thus is smaller than c in magnitude. Integrating the equations of motion Schrödinger found

$$\begin{aligned} \hat{\boldsymbol{x}}(t) &= \hat{U}_0(t)^* \hat{\boldsymbol{x}} \hat{U}_0(t) \\ &= \hat{\boldsymbol{x}}(0) + c^2 \hat{\boldsymbol{p}} \hat{H}_0^{-1} t + \frac{\hbar}{2\mathrm{i}} \hat{H}_0^{-1} \big(\mathrm{e}^{\frac{2\mathrm{i}}{\hbar}\hat{H}_0 t} - 1\big) \hat{\boldsymbol{F}}. \end{aligned} \tag{2.2}$$

The first two terms of this result exactly correspond to the respective classical dynamics of a free relativistic particle. The third term, however, contains the operator

$$\hat{\boldsymbol{F}} := c\boldsymbol{\alpha} - c^2 \hat{\boldsymbol{p}} \hat{H}_0^{-1}$$

which is well defined since zero is not in the spectrum of $\hat{H}_0$ and thus $\hat{H}_0^{-1}$ is a bounded operator. The quantity $\hat{\boldsymbol{F}}$ expresses the difference between the velocity operator and the quantization of the classical velocity. This additional term introduces a rapidly oscillating time dependence and hence was named *Zitterbewegung (trembling motion)* by Schrödinger.

After Schrödinger's work [Sch30] the origin of the Zitterbewegung was traced back to the coexistence of particles and anti-particles in relativistic quantum mechanics. Therefore, this effect can be removed by projecting the standard position operator to the particle and anti-particle subspaces of $\mathscr{H}$, respectively. To this end one introduces the projection operators

$$\hat{P}_0^\pm := \tfrac{1}{2}(\mathbb{1}_{\mathscr{H}} \pm |\hat{H}_0|^{-1} \hat{H}_0) \tag{2.3}$$

with $|\hat{H}_0| := (\hat{H}_0^* \hat{H}_0)^{1/2}$, fulfilling $\hat{P}_0^+ \hat{P}_0^- = 0$ and $\hat{P}_0^+ + \hat{P}_0^- = \mathbb{1}_{\mathscr{H}}$. The time evolution of the projected position operators

$$\hat{\boldsymbol{x}}_0^\pm := \hat{P}_0^\pm \hat{\boldsymbol{x}} \hat{P}_0^\pm \tag{2.4}$$

is then given by (see [Tha92])

$$\hat{\boldsymbol{x}}_0^\pm(t) = \hat{\boldsymbol{x}}_0^\pm(0) + c^2 \hat{\boldsymbol{p}} \hat{H}_0^{-1} t \hat{P}_0^\pm.$$

It hence exactly corresponds to the respective classical expression; and this is true for both particles and anti-particles. The interpretation of this observation is obvious: particles and anti-particles show noticeably different time evolutions and the Zitterbewegung in (2.2) represents the interference term [Tha92]

$$\hat{P}_0^+ \hat{\boldsymbol{x}} \hat{P}_0^- + \hat{P}_0^- \hat{\boldsymbol{x}} \hat{P}_0^+ = \frac{\mathrm{i}\hbar}{2} \hat{H}_0^{-1} \hat{\boldsymbol{F}}$$

that is absent in a classical description.

We remark that the projected position operators (2.4) differ from the Newton–Wigner position operators introduced in [NW49]. Whereas the latter also respect the splitting of the Hilbert space into particle and anti-particle subspaces, they arise from the standard position operator by unitary transformations. The Newton–Wigner operators are unique in the sense that they possess certain natural localization properties [Wig62]. However, it is well known that in relativistic quantum mechanics no position operators exist that leave the particle and anti-particle subspaces invariant, share the natural localization properties and do not violate Einstein causality; see, e.g., the discussion in [Tha92]. Thus even for free particles no complete quantum–classical correspondence exists. The goal we want to achieve in the following hence is to promote a method that allows us to separate particles from anti-particles in a semiclassical fashion: the Hilbert space is split into mutually orthogonal subspaces and observables are projected to these subspaces. Within these subspaces one can then employ semiclassical techniques and set up quantum–classical correspondences. In the following section we are going to extend this concept to particles interacting with external fields. In this situation even a separation of $\mathscr{H}$ into subspaces that are associated with particles and anti-particles, respectively, can only be achieved asymptotically (in the semiclassical limit).

3. Semiclassical projection operators

We now consider the Dirac equation

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

for a particle of mass m and charge e coupled to external time-independent electromagnetic fields $\boldsymbol{E}(\boldsymbol{x}) = -\mathrm{grad}\,\phi(\boldsymbol{x})$ and $\boldsymbol{B}(\boldsymbol{x}) = \mathrm{rot}\,\boldsymbol{A}(\boldsymbol{x})$. The Hamiltonian therefore reads

$$\hat{H} = c\boldsymbol{\alpha}\cdot\left(\frac{\hbar}{\mathrm{i}}\nabla - \frac{e}{c}\boldsymbol{A}(\boldsymbol{x})\right) + \beta mc^2 + e\phi(\boldsymbol{x}). \tag{3.1}$$

For convenience we restrict our attention to smooth potentials, in which case the operator (3.1) is known to be essentially self-adjoint on the domain $C_0^\infty(\mathbb{R}^3)\otimes\mathbb{C}^4$ (see, e.g., [Tha92]) and hence defines a unitary time evolution

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

In order to separate particles and anti-particles also in the presence of electromagnetic fields one would like to construct projection operators analogous to (2.3) that commute with the Hamiltonian. This, however, is not possible as can be seen by considering operators in a phase-space representation. Here we choose the Wigner–Weyl calculus in which an operator $\hat{B}$ on $\mathscr{H}$ is defined in terms of a function $B(\boldsymbol{x},\boldsymbol{p})$ on phase space taking values in the 4×4 matrices,

$$(\hat{B}\psi)(\boldsymbol{x}) = \frac{1}{(2\pi\hbar)^3}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})} B\left(\frac{\boldsymbol{x}+\boldsymbol{y}}{2},\boldsymbol{p}\right)\psi(\boldsymbol{y})\,\mathrm{d}y\,\mathrm{d}p. \tag{3.2}$$

This operator is well defined on Dirac spinors $\psi\in\mathscr{S}(\mathbb{R}^3)\otimes\mathbb{C}^4$, if the matrix-valued Weyl symbol $B(\boldsymbol{x},\boldsymbol{p})$ is smooth. For this and further details of the Weyl calculus see [Fol89, Rob87, DS99]. Introducing then, e.g., the symbol

$$H(\boldsymbol{x},\boldsymbol{p}) = c\boldsymbol{\alpha}\cdot\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}(\boldsymbol{x})\right) + \beta mc^2 + e\phi(\boldsymbol{x}) \tag{3.3}$$

one can represent the Hamiltonian (3.1) as a Weyl operator (3.2). For each point $(\boldsymbol{x},\boldsymbol{p})$ in phase space the symbol (3.3) is a Hermitian 4×4 matrix with the two doubly degenerate eigenvalues

$$h_\pm(\boldsymbol{x},\boldsymbol{p}) = e\phi(\boldsymbol{x}) \pm \sqrt{(c\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{x}))^2 + m^2c^4}. \tag{3.4}$$

These functions can immediately be identified as the classical Hamiltonians of particles and anti-particles, respectively, without spin. Associated with these eigenvalues are the projection matrices

$$\Pi_0^{\pm}(\boldsymbol{x},\boldsymbol{p}) = \frac{1}{2}\left(\mathbb{1}_4 \pm \frac{\boldsymbol{\alpha}\cdot(c\boldsymbol{p}-e\boldsymbol{A}(\boldsymbol{x}))+\beta mc^2}{\sqrt{(c\boldsymbol{p}-e\boldsymbol{A}(\boldsymbol{x}))^2+m^2c^4}}\right) \tag{3.5}$$

onto the respective eigenspaces in $\mathbb{C}^4$. In the absence of potentials the matrix-valued functions (3.5) are independent of $\boldsymbol{x}$ and their Weyl quantizations according to (3.2) yield the projectors (2.3). One could hence be tempted to view the Weyl quantizations $\hat{\Pi}_0^{\pm}$ of the symbols (3.5) as appropriate substitutes for the operators (2.3) in the general case. Indeed, if the partial derivatives of $\boldsymbol{A}(\boldsymbol{x})$ are bounded, the quantities (3.5) and all their partial derivatives are bounded smooth functions of $(\boldsymbol{x},\boldsymbol{p})$ such that the operators $\hat{\Pi}_0^{\pm}$ are self-adjoint and bounded on the Hilbert space $\mathscr{H}$ [CV71]. The fact that the symbols (3.5) depend on $\boldsymbol{x}$, however, implies that $\hat{\Pi}_0^{\pm}$ are not projection operators, but satisfy [EW96]

$$\left(\hat{\Pi}_0^{\pm}\right)^2 - \hat{\Pi}_0^{\pm} = O(\hbar). \tag{3.6}$$

Moreover, $\hat{\Pi}_0^{\pm}$ do not commute with the Hamiltonian.

The error on the right-hand side of (3.6) can be improved by adding a suitable term of order $\hbar$ to the symbol (3.5). To guarantee that the Weyl quantization of this symbol leads to a bounded operator, we now require that the potential $\phi(\boldsymbol{x})$ and all its partial derivatives are bounded, and that $\boldsymbol{A}(\boldsymbol{x})$ grows at most like some power $|\boldsymbol{x}|^K$. In this case the quantity

$$\varepsilon(\boldsymbol{x},\boldsymbol{p}) := \sqrt{(c\boldsymbol{p}-e\boldsymbol{A}(\boldsymbol{x}))^2+m^2c^4} \tag{3.7}$$

may serve as a so-called order function for the symbol (3.3) and the construction of [BG04] applies. After quantization of the corrected symbol this leads to an operator that is a projector up to an error of order $\hbar^2$. This procedure can be repeated to an arbitrary order $\hbar^N$, see [EW96, BN99]. One hence obtains almost projection operators $\hat{\Pi}^{\pm}$ that almost commute with the Hamiltonian,

$$(\hat{\Pi}^{\pm})^2 - \hat{\Pi}^{\pm} = O(\hbar^{\infty}) \qquad \text{and} \qquad [\hat{H},\hat{\Pi}^{\pm}] = O(\hbar^{\infty}) \tag{3.8}$$

meaning that the operator norm of the above expressions is smaller than any power of $\hbar$. Furthermore,

$$\hat{\Pi}^{+}\hat{\Pi}^{-} = O(\hbar^{\infty}) \qquad \text{and} \qquad \hat{\Pi}^{+}+\hat{\Pi}^{-} = \mathbb{1}_{\mathscr{H}} + O(\hbar^{\infty}). \tag{3.9}$$

As a consequence of $\hat{\Pi}^{\pm}$ being almost projectors, their spectrum is concentrated around zero and one. The standard Riesz projection formula therefore allows us to construct the genuine orthogonal projectors

$$\hat{P}^{\pm} := \frac{1}{2\pi\mathrm{i}}\int_{|\lambda-1|=\frac{1}{2}} (\hat{\Pi}^{\pm}-\lambda)^{-1}\,\mathrm{d}\lambda$$

which also almost commute with $\hat{H}$ and fulfil (3.9).

Since the above construction is based on the separation into particles and anti-particles on a classical level (3.4) and is then extended order by order in $\hbar$, one can view the subspaces $\mathscr{H}^{\pm} := \hat{P}^{\pm}\mathscr{H}$ as being semiclassically associated with particles and anti-particles, respectively. Moreover, due to relation (3.8) these subspaces are almost invariant with respect to the time evolution generated by $\hat{H}$, i.e.

$$\hat{U}(t)\hat{P}^{\pm}\psi - \hat{P}^{\pm}\hat{U}(t)\psi = O(t\hbar^{\infty}) \qquad \text{for all} \quad \psi \in \mathscr{H}.$$

Hence, up to a small error every spinor in one of the subspaces $\mathscr{H}^{\pm}$ remains under the time evolution within this subspace; and this is true for semiclassically long times $t \ll \hbar^{-N}$, where

N can be chosen arbitrarily large. This result is in agreement with the (heuristic) physical picture that particles interact with anti-particles via tunnelling; the latter is a genuine quantum process with pair production and annihilation rates that are exponentially small in $\hbar$. Related to this observation is the fact that eigenspinors of the Hamiltonian can (only) almost be associated with particles or anti-particles: If $\psi_n \in \mathscr{H}$ is an eigenspinor, $\hat{H}\psi_n = E_n\psi_n$, its projections $\hat{P}^{\pm}\psi_n$ are in general only almost eigenspinors (quasimodes), i.e.

$$(\hat{H} - E_n)\hat{P}^{\pm}\psi_n = O(\hbar^{\infty}).$$

Thus the discrete spectrum of the Hamiltonian cannot truly be divided into a particle and an anti-particle part. Further consequences will be investigated in section 6.

The above discussion raises the question whether the semiclassical projectors $\hat{P}^{\pm}$ can (at least semiclassically) be related to spectral projections of the Hamiltonian. According to (2.3), in the case without potentials the operators $\hat{P}_0^{\pm}$ are obviously the spectral projectors to $(-\infty, -mc^2)$ and (mc^2, ∞), which are exactly the (absolutely continuous) spectral stretches associated with particles and anti-particles, respectively. In the presence of potentials, depending on their behaviour at infinity, there exist constants $E_+ > E_-$ such that the spectrum inside (E_-, E_+) is discrete and absolutely continuous outside; e.g., if the potentials and their derivatives vanish at infinity one finds $E_{\pm} = \pm mc^2$, see [Tha92]. For $E \in (E_-, E_+)$ not in the spectrum of $\hat{H}$ we then denote the spectral projectors to $(-\infty, E)$ and (E, ∞) by $\hat{P}_E^-$ and $\hat{P}_E^+$, respectively. For the rest of this section we also assume that

$$h_-(\boldsymbol{x}, \boldsymbol{p}) < E < h_+(\boldsymbol{x}, \boldsymbol{p}) \quad \text{for all } (\boldsymbol{x}, \boldsymbol{p})$$

i.e., the classical particle and anti-particle Hamiltonians are separated by a gap as $(\boldsymbol{x}, \boldsymbol{p})$ runs over phase space. Therefore, the two classical energy shells

$$\Omega_E^{\pm} = \{(\boldsymbol{x}, \boldsymbol{p}); h_{\pm}(\boldsymbol{x}, \boldsymbol{p}) = E\}$$

are empty and, moreover, for any value E' at least one of the energy shells $\Omega_{E'}^{\pm}$ is empty. On the submanifold $\boldsymbol{p} = \frac{e}{c}\boldsymbol{A}(\boldsymbol{x})$ this condition requires that the variation of the potential $\phi(\boldsymbol{x})$ is strictly restricted by $2mc^2$. In such a situation the semiclassical projectors $\hat{P}^{\pm}$ are semiclassically close to the spectral projectors,

$$\left\| \hat{P}^{\pm} - \hat{P}_E^{\pm} \right\| = O(\hbar^{\infty}).$$

A full proof of this statement can be found in [BG04].

4. Semiclassical observables

The example of the standard position operator for the free particle and its Zitterbewegung demonstrates that not all quantum observables possess a direct (semi-) classical interpretation. Only the diagonal blocks with respect to the projections $\hat{P}_0^{\pm}$ allow for establishing quantum–classical correspondences. This observation applies in particular to dynamical questions because only after projection there exists an unambiguous classical Hamiltonian (3.4). Following the discussion in the previous section, these remarks carry over to the general case appropriately. Our aim therefore is to identify a sufficiently large class of observables with a semiclassical meaning. We moreover require this class to be invariant with respect to the quantum time evolution, i.e. $\hat{B}$ being of this class should imply that $\hat{B}(t) = \hat{U}(t)^*\hat{B}\hat{U}(t)$ is of the same type.

A natural starting point in the present context is to choose the Weyl representation (3.2) for operators on $\mathscr{H}$. It is well known that this is possible for a fairly large class of operators, namely those that are continuous from $\mathscr{S}(\mathbb{R}^3 \times \mathbb{R}^3) \otimes \mathbb{C}^4$ to $\mathscr{S}'(\mathbb{R}^3 \times \mathbb{R}^3) \otimes \mathbb{C}^4$; see, e.g., [Fol89, DS99]. In order to achieve manageable algebraic properties, however, one must restrict the class of operators further. For convenience we here choose Weyl quantizations of smooth symbols $B(\boldsymbol{x}, \boldsymbol{p})$ that are, along with all of their partial derivatives, bounded on $\mathbb{R}^3 \times \mathbb{R}^3$. This restriction leads to bounded operators on $\mathscr{H}$, see [CV71]. We admit $\hbar$-dependent symbols, since even when restricting to quantizations $\hat{B}$ of $\hbar$-independent symbols $B(\boldsymbol{x}, \boldsymbol{p})$ their time evolutions $\hat{B}(t)$ will necessarily acquire an $\hbar$-dependence in their symbols $B(t)(\boldsymbol{x}, \boldsymbol{p}; \hbar)$. But for the purpose of convenient semiclassical asymptotics we restrict the $\hbar$-dependence in a particular way,

$$B(\boldsymbol{x}, \boldsymbol{p}; \hbar) \sim \sum_{k=0}^{\infty} \hbar^k B_k(\boldsymbol{x}, \boldsymbol{p}). \tag{4.1}$$

The asymptotic expansion is to be understood in the sense that

$$\left\| \partial_x^\alpha \partial_p^\beta \left(B(\boldsymbol{x}, \boldsymbol{p}; \hbar) - \sum_{k=0}^{N-1} \hbar^k B_k(\boldsymbol{x}, \boldsymbol{p}) \right) \right\|_{4\times 4} \leqslant C_{\alpha,\beta}^{(N)} \hbar^N \tag{4.2}$$

holds for all $(\boldsymbol{x}, \boldsymbol{p}) \in \mathbb{R}^3 \times \mathbb{R}^3$ and all $N \in \mathbb{N}$ uniformly in $\hbar$ as $\hbar \to 0$, where $\|\cdot\|_{4\times 4}$ denotes an arbitrary matrix norm. We call the quantizations of such symbols semiclassical observables. These form a subalgebra $\mathcal{O}_{\mathrm{sc}}$ in the algebra of bounded operators on $\mathscr{H}$. As usual, only the self-adjoint elements of $\mathcal{O}_{\mathrm{sc}}$ are true quantum mechanical observables; they can be characterized by symbols taking values in the Hermitian 4×4 matrices.

The crucial point now is to identify a subalgebra $\mathcal{O}_{\mathrm{inv}}$ in $\mathcal{O}_{\mathrm{sc}}$ that is invariant with respect to the quantum time evolution. We recall that in the case of scalar operators, such as Schrödinger–Hamiltonians on $L^2(\mathbb{R}^3)$, the respective algebra $\mathcal{O}_{\mathrm{sc}}$ itself is invariant; see, e.g., [Rob87]. The Zitterbewegung of a free relativistic particle, however, shows that in the present context this can no longer hold. This example also suggests that $\mathcal{O}_{\mathrm{inv}}$ might consist of those semiclassical observables that are block-diagonal with respect to the semiclassical projections $\hat{P}^\pm$. In the following we are going to demonstrate that this is indeed the case.

Since the necessary constructions take place in terms of symbols, we first recall how the algebraic properties of semiclassical observables are reflected on this level; see, e.g., [Fol89, Rob87, DS99]: the product of two semiclassical observables $\hat{B}, \hat{C} \in \mathcal{O}_{\mathrm{sc}}$ is a Weyl operator with a symbol denoted by $B\#C(\boldsymbol{x}, \boldsymbol{p}; \hbar)$. This symbol has an asymptotic expansion of the type (4.1) and (4.2) that reads

$$B\#C(\boldsymbol{x}, \boldsymbol{p}; \hbar) \sim \sum_{j,k,l=0}^{\infty} \frac{\hbar^{j+k+l}}{j!} \left(\frac{\mathrm{i}}{2} (\nabla_x \cdot \nabla_\xi - \nabla_p \cdot \nabla_y) \right)^j B_k(\boldsymbol{p}, \boldsymbol{x}) C_l(\boldsymbol{\xi}, \boldsymbol{y}) \bigg|_{\substack{\boldsymbol{y}=\boldsymbol{x} \\ \boldsymbol{\xi}=\boldsymbol{p}}}.$$

We remark that if the operator $\hat{C}$ is replaced by the Hamiltonian $\hat{H}$ a corresponding product formula for the symbol $B\#H(\boldsymbol{x}, \boldsymbol{p}; \hbar)$ exists, with the exception that on the right-hand side of the estimates (4.2) the order function (3.7) appears as an additional factor.

We are now in a position to write down the Heisenberg equation of motion for the time evolution $\hat{B}(t)$ of a semiclassical observable in terms of symbols,

$$\frac{\partial}{\partial t} B(t)(\boldsymbol{x}, \boldsymbol{p}; \hbar) = \frac{\mathrm{i}}{\hbar} (H\#B(t) - B(t)\#H)(\boldsymbol{x}, \boldsymbol{p}; \hbar). \tag{4.3}$$

The strategy we follow now is to assume an asymptotic expansion of the form (4.2) for the symbol $B(t)(\boldsymbol{x}, \boldsymbol{p}; \hbar)$, insert this into (4.3) and solve, if possible, the hierarchy of equations for the coefficients $B(t)_k(\boldsymbol{x}, \boldsymbol{p})$ of $\hbar^k$. A first obstacle to this procedure arises upon investigating the leading terms on the right-hand side of (4.3),

$$\frac{\partial}{\partial t} B(t) = \frac{\mathrm{i}}{\hbar} [H, B(t)_0] - \frac{1}{2} (\{H, B(t)_0\} - \{B(t)_0, H\}) + \mathrm{i}[H, B(t)_1] + O(\hbar). \tag{4.4}$$

Here $[\cdot,\cdot]$ is a matrix commutator and

$$\{B, C\}(\boldsymbol{x}, \boldsymbol{p}) = (\nabla_p B \cdot \nabla_x C - \nabla_x B \cdot \nabla_p C)(\boldsymbol{x}, \boldsymbol{p})$$

denotes the Poisson bracket for matrix-valued functions on phase space. Due to the factor of $1/\hbar$ in the first term on the right-hand side of (4.4) the proposed strategy can only be consistent if the matrix-valued function $B(t)_0(\boldsymbol{x}, \boldsymbol{p})$ is block-diagonal with respect to the eigenprojections $\Pi_0^{\pm}(\boldsymbol{x}, \boldsymbol{p})$ of the symbol matrix $H(\boldsymbol{x}, \boldsymbol{p})$. This condition is the lowest semiclassical order of the expected restriction on the operators in $\mathcal{O}_{\text{inv}}$.

Necessary and sufficient conditions to be imposed on semiclassical observables to be in $\mathcal{O}_{\text{inv}}$ can be obtained in any semiclassical order, if the solvability of equations (4.3) for the diagonal and for the off-diagonal blocks of $B(t)$ with respect to the projection symbols $\Pi^{\pm}$ are investigated. This leads to the following.

Theorem 4.1. *A semiclassical observable $\hat{B} \in \mathcal{O}_{\text{sc}}$ lies in the invariant algebra $\mathcal{O}_{\text{inv}}$, if and only if its off-diagonal blocks with respect to the semiclassical projections $\hat{P}^{\pm}$ are smaller than any power of $\hbar$,*

$$\hat{P}^{\pm}\hat{B}\hat{P}^{\mp} = O(\hbar^{\infty}). \tag{4.5}$$

This statement is a version appropriate for the Dirac equation of a result proved in [BG04].

The Hamiltonian (3.1) is not in $\mathcal{O}_{\text{inv}}$, but this is only due to our restriction to bounded operators; otherwise, relations (3.8) and (3.9) imply that $\hat{H}$ indeed possesses the property (4.5). Furthermore, up to errors of the order $\hbar^{\infty}$ the time evolution of the diagonal blocks $\hat{P}^{\pm}\hat{B}\hat{P}^{\pm}$ is governed by the projected Hamiltonians $\hat{H}\hat{P}^{\pm}$. An interpretation of theorem 4.1 now is rather obvious: an observable remains semiclassical under the quantum dynamics if it does not contain off-diagonal blocks representing an interference of particle and anti-particle dynamics, since this has no classical equivalent. Terms exceptional to this must be smaller than any power of $\hbar$, indicating that they arise from pure quantum effects.

5. Classical limit of quantum dynamics

Given an observable $\hat{B} \in \mathcal{O}_{\text{inv}}$, we are interested in the connection between its time evolution $\hat{B}(t)$ and appropriate classical dynamics. The diagonal blocks of $\hat{B}$ are (approximately) propagated with the projected Hamiltonians $\hat{H}\hat{P}^{\pm}$, whose symbols read

$$H(\boldsymbol{x}, \boldsymbol{p})\Pi_0^{\pm}(\boldsymbol{x}, \boldsymbol{p}) = h_{\pm}(\boldsymbol{x}, \boldsymbol{p})\Pi_0^{\pm}(\boldsymbol{x}, \boldsymbol{p})$$

to leading order. We therefore expect the equations of motion generated by the eigenvalue functions (3.4),

$$\dot{\boldsymbol{x}}_{\pm}(t) = \{h_{\pm}, \boldsymbol{x}_{\pm}(t)\} \qquad \dot{\boldsymbol{p}}_{\pm}(t) = \{h_{\pm}, \boldsymbol{p}_{\pm}(t)\} \tag{5.1}$$

to play an important role for the classical limit of the quantum time evolution. The solutions to (5.1) define the Hamiltonian flows $\Phi_{\pm}^{t}(\boldsymbol{p}, \boldsymbol{x}) = (\boldsymbol{p}_{\pm}(t), \boldsymbol{x}_{\pm}(t))$, with $(\boldsymbol{p}_{\pm}(0), \boldsymbol{x}_{\pm}(0)) = (\boldsymbol{p}, \boldsymbol{x})$, on phase space. These flows represent the classical dynamics of relativistic particles (and anti-particles). Spin is absent from these expressions, reflecting the fact that *a priori* spin is a quantum mechanical concept and its classical counterpart has to be recovered in systematic semiclassical approximations of the quantum system.

In the present situation the kinematics and the dynamics of spin are encoded in the matrix part of the symbols of observables. For an observable $\hat{B} \in \mathcal{O}_{\text{inv}}$ the leading semiclassical order of its symbol is composed of the functions

$$\left(\Pi_0^{\pm} B_0 \Pi_0^{\pm}\right)(\boldsymbol{x}, \boldsymbol{p}) \tag{5.2}$$

taking values in the (Hermitian) 4×4 matrices. These matrices act on the two-dimensional subspaces $\Pi_0^{\pm}(\boldsymbol{x}, \boldsymbol{p})\mathbb{C}^4$ of $\mathbb{C}^4$, which can be viewed as Hilbert spaces of a spin $1/2$ attached to a classical particle or anti-particle, respectively, at the point $(\boldsymbol{x}, \boldsymbol{p})$ in phase space. In order to work in these two-dimensional spaces explicitly, one can introduce orthonormal bases $\left\{e_1^{\pm}(\boldsymbol{x}, \boldsymbol{p}), e_2^{\pm}(\boldsymbol{x}, \boldsymbol{p})\right\}$ for each of them. For convenience the vectors $e_k^{\pm}(\boldsymbol{x}, \boldsymbol{p}) \in \mathbb{C}^4$ are chosen as eigenvectors of the symbol matrix $H(\boldsymbol{x}, \boldsymbol{p})$ with eigenvalues $h_{\pm}(\boldsymbol{x}, \boldsymbol{p})$. Upon expanding vectors from $\Pi_0^{\pm}(\boldsymbol{x}, \boldsymbol{p})\mathbb{C}^4$ in these bases one introduces isometries $V_{\pm}(\boldsymbol{x}, \boldsymbol{p})$: $\mathbb{C}^2 \to \Pi_0^{\pm}(\boldsymbol{x}, \boldsymbol{p})\mathbb{C}^4$, such that $V_{\pm}(\boldsymbol{x}, \boldsymbol{p})V_{\pm}^*(\boldsymbol{x}, \boldsymbol{p}) = \Pi_0^{\pm}(\boldsymbol{x}, \boldsymbol{p})$ and $V_{\pm}^*(\boldsymbol{x}, \boldsymbol{p})V_{\pm}(\boldsymbol{x}, \boldsymbol{p}) = \mathbb{1}_2$. A possible choice for these isometries is

$$V_+(\boldsymbol{x}, \boldsymbol{p}) = \frac{1}{\sqrt{2\varepsilon(\boldsymbol{x}, \boldsymbol{p})(\varepsilon(\boldsymbol{x}, \boldsymbol{p}) + mc^2)}} \begin{pmatrix} (\varepsilon(\boldsymbol{x}, \boldsymbol{p}) + mc^2)\mathbb{1}_2 \\ (c\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{x})) \cdot \boldsymbol{\sigma} \end{pmatrix}$$

$$V_-(\boldsymbol{x}, \boldsymbol{p}) = \frac{1}{\sqrt{2\varepsilon(\boldsymbol{x}, \boldsymbol{p})(\varepsilon(\boldsymbol{x}, \boldsymbol{p}) + mc^2)}} \begin{pmatrix} (c\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{x})) \cdot \boldsymbol{\sigma} \\ -(\varepsilon(\boldsymbol{x}, \boldsymbol{p}) + mc^2)\mathbb{1}_2 \end{pmatrix}.$$

That way the diagonal blocks (5.2) can be represented in terms of the 2×2 matrices

$$\left(V_{\pm}^* B_0 V_{\pm}\right)(\boldsymbol{x}, \boldsymbol{p}) \tag{5.3}$$

which are Hermitian if $B_0(\boldsymbol{x}, \boldsymbol{p})$ is Hermitian on $\mathbb{C}^4$.

The matrix-valued functions (5.3) can be mapped in a one–to–one manner to real-valued functions on the sphere S^2 via

$$b_0^{\pm}(\boldsymbol{x}, \boldsymbol{p}, \boldsymbol{n}) := \tfrac{1}{2}\,\mathrm{tr}\big(\Delta_{1/2}(\boldsymbol{n})\big(V_{\pm}^* B_0 V_{\pm}\big)(\boldsymbol{x}, \boldsymbol{p})\big) \tag{5.4}$$

where $\boldsymbol{n} \in \mathbb{R}^3$ with $|\boldsymbol{n}| = 1$ is viewed as a point on S^2 and

$$\Delta_{1/2}(\boldsymbol{n}) := \tfrac{1}{2}(\mathbb{1}_2 + \sqrt{3}\boldsymbol{n} \cdot \boldsymbol{\sigma})$$

takes values in the Hermitian 2×2 matrices, see [VGB89]. The quantizers $\Delta_{1/2}(\boldsymbol{n})$ provide a quantum–classical correspondence on the sphere that is covariant with respect to $SU(2)$ rotations in the following sense:

$$g\Delta_{1/2}(\boldsymbol{n})g^{-1} = \Delta_{1/2}(R(g)\boldsymbol{n}). \tag{5.5}$$

Here $R(g) \in SO(3)$ is a rotation associated with $g \in SU(2)$ through $g\boldsymbol{n}\cdot\boldsymbol{\sigma}g^{-1} = (R(g)\boldsymbol{n})\cdot\boldsymbol{\sigma}$; see [BGK01] for further details. The semiclassically leading term of a (block-diagonal) semiclassical observable $\hat{B}$ can therefore be represented by two real-valued functions on the space $\mathbb{R}^3 \times \mathbb{R}^3 \times \mathrm{S}^2$. Through the relation

$$(V_{\pm}^* B_0 V_{\pm})(\boldsymbol{x}, \boldsymbol{p}) = \int_{\mathrm{S}^2} b_0^{\pm}(\boldsymbol{x}, \boldsymbol{p}, \boldsymbol{n})\Delta_{1/2}(\boldsymbol{n})\,\mathrm{d}\boldsymbol{n}$$

where $\mathrm{d}\boldsymbol{n}$ is the normalized area form on S^2, the matrix-valued expressions (5.3) are unambiguously recovered from the functions (5.4) [BGK01].

The point $\boldsymbol{n} \in \mathrm{S}^2$ that arises as an additional variable in a general classical observable (5.4) can be viewed as a classical equivalent of spin. This interpretation is suggested by the fact that the classical observable (5.4) associated with quantum spin,

$$\hat{B} = \frac{\hbar}{2}\Sigma_k \qquad \text{with} \quad \Sigma_k := \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}$$

can be calculated as

$$\begin{aligned} b_0^{\pm}(\boldsymbol{x}, \boldsymbol{p}, \boldsymbol{n}) &= \frac{\hbar}{2}\,\mathrm{tr}(\Delta_{1/2}(\boldsymbol{n})V_{\pm}^*(\boldsymbol{x}, \boldsymbol{p})\Sigma_k V_{\pm}(\boldsymbol{x}, \boldsymbol{p})) \\ &= \sqrt{\frac{1}{2}\left(\frac{1}{2} + 1\right)}\hbar n_k. \end{aligned}$$

Up to its normalization, which depends on $\hbar$ and the spin quantum number $s = 1/2$, the point $\boldsymbol{n} \in \mathrm{S}^2$ can thus be considered as a classical spin. The latter is therefore represented on its natural phase space S^2, and the space $\mathbb{R}^3 \times \mathbb{R}^3 \times \mathrm{S}^2$ on which the classical observables (5.4) are defined can be viewed as the combined phase space of the translational and the spin degrees of freedom.

We now want to identify the classical dynamics of both the translational and the spin degrees of freedom that emerge in the semiclassical limit of the quantum dynamics generated by the Hamiltonian $\hat{H}$. To this end we recall that $\mathcal{O}_{\mathrm{inv}}$ was defined to contain those semiclassical observables $\hat{B} \in \mathcal{O}_{\mathrm{sc}}$ whose time evolutions $\hat{B}(t) = \hat{U}(t)^*\hat{B}\hat{U}(t)$ are again semiclassical observables. Hence $\hat{B}(t)$ is a Weyl operator of the form (3.2) with symbol $B(t)(\boldsymbol{x}, \boldsymbol{p}; \hbar)$ that possesses an asymptotic expansion of the type (4.1). The leading term $B(t)_0(\boldsymbol{x}, \boldsymbol{p})$ in this expansion then yields the classical time evolution of both types of degrees of freedom.

Theorem 5.1. *When $\hat{B} \in \mathcal{O}_{\mathrm{inv}}$ the semiclassically leading term in the asymptotic expansion of the symbol of its time evolution $\hat{B}(t)$ reads*

$$B(t)_0(\boldsymbol{x}, \boldsymbol{p}) = \sum_{\nu \in \{+,-\}} d_\nu^*(\boldsymbol{x}, \boldsymbol{p}, t)\big(\Pi_0^\nu B_0 \Pi_0^\nu\big)\big(\Phi_\nu^t(\boldsymbol{x}, \boldsymbol{p})\big) d_\nu(\boldsymbol{x}, \boldsymbol{p}, t). \tag{5.6}$$

The unitary 4×4 matrices $d_\pm(\boldsymbol{x}, \boldsymbol{p}, t)$ are determined by the transport equations

$$\dot{d}_\pm(\boldsymbol{x}, \boldsymbol{p}, t) + \mathrm{i} H_\pm\big(\Phi_\pm^t(\boldsymbol{x}, \boldsymbol{p})\big) d_\pm(\boldsymbol{p}, \boldsymbol{x}, t) = 0 \qquad d_\pm(\boldsymbol{p}, \boldsymbol{x}, 0) = 1_4 \tag{5.7}$$

where the effective spin-Hamiltonians $H_\pm$ are defined as

$$H_\pm := -\mathrm{i}\big[\Pi_0^\pm, \big\{h_\pm, \Pi_0^\pm\big\}\big] + \frac{\mathrm{i}}{2}\big(h_\pm \Pi_0^\pm \big\{\Pi_0^\pm, \Pi_0^\pm\big\}\Pi_0^\pm + \Pi_0^\pm\big\{\Pi_0^\pm, H - h_\pm \Pi_0^\pm\big\}\Pi_0^\pm\big). \tag{5.8}$$

We refrain from giving explicit expressions for the 4×4 effective spin-Hamiltonians (5.8) here since below we will only work in a 2×2 representation; instead we refer to [Spo00]. A statement of the type made in theorem 5.1 is usually called an Egorov theorem [Ego69]. The present version is covered by the Egorov theorem in [BG04], where one can also find a proof.

The 4×4 matrices $d_\pm(\boldsymbol{x}, \boldsymbol{p}, t)$ can be shown to map the two-dimensional subspaces $\Pi_0^\pm(\boldsymbol{x}, \boldsymbol{p})\mathbb{C}^4$ of $\mathbb{C}^4$ unitarily to the propagated subspaces $\Pi_0^\pm\big(\Phi_\pm^t(\boldsymbol{x}, \boldsymbol{p})\big)\mathbb{C}^4$ [BG04]. They hence describe the transport of the (anti-) particle spin along the classical trajectories $(\boldsymbol{x}_\pm(t), \boldsymbol{p}_\pm(t))$. If one prefers to work in the orthonormal eigenbases $\big\{\mathrm{e}_1^\pm(\boldsymbol{x}, \boldsymbol{p}), \mathrm{e}_2^\pm(\boldsymbol{x}, \boldsymbol{p})\big\}$ of the spaces $\Pi_0^\pm(\boldsymbol{x}, \boldsymbol{p})\mathbb{C}^4$ one can introduce the unitary 2×2 matrices

$$D_\pm(\boldsymbol{x}, \boldsymbol{p}, t) := V_\pm^*\big(\Phi_\pm^t(\boldsymbol{x}, \boldsymbol{p})\big) d_\pm(\boldsymbol{x}, \boldsymbol{p}, t) V_\pm(\boldsymbol{x}, \boldsymbol{p})$$

which are determined by the equations

$$\dot{D}_\pm(\boldsymbol{x}, \boldsymbol{p}, t) + \frac{\mathrm{i}}{2}\boldsymbol{C}_\pm\big(\Phi_\pm^t(\boldsymbol{x}, \boldsymbol{p})\big) \cdot \boldsymbol{\sigma} D_\pm(\boldsymbol{p}, \boldsymbol{x}, t) = 0 \qquad D_\pm(\boldsymbol{p}, \boldsymbol{x}, 0) = 1_2 \tag{5.9}$$

following from (5.7). The transformed effective spin-Hamiltonians $\boldsymbol{C}_\pm \cdot \boldsymbol{\sigma}/2$ derive from (5.8) and can be expressed in terms of the electromagnetic fields through

$$\boldsymbol{C}_\pm(\boldsymbol{x}, \boldsymbol{p}) = \mp\frac{ec}{\varepsilon(\boldsymbol{x}, \boldsymbol{p})}\left(\boldsymbol{B}(\boldsymbol{x}) \pm \frac{1}{\varepsilon(\boldsymbol{x}, \boldsymbol{p}) + mc^2}(c\boldsymbol{E}(\boldsymbol{x}) \times (c\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{x})))\right)$$

where $\varepsilon(\boldsymbol{x}, \boldsymbol{p})$ is defined in (3.7). Since therefore the effective spin-Hamiltonians are Hermitian and traceless 2×2 matrices, the solutions $D_\pm$ of (5.9) are in $SU(2)$. Related results have previously been obtained in a WKB–type situation [RK63, BK98, BK99] and in the context of a semiclassical propagation of Wigner functions [Spo00].

The transport matrices $D_\pm(\boldsymbol{x}, \boldsymbol{p}, t)$ carry two-component spinors along the trajectories $\Phi_\pm^t(\boldsymbol{x}, \boldsymbol{p})$ and induce a classical spin dynamics along (anti-) particle trajectories. These combined classical dynamics can be recovered upon representing the leading symbol (5.6) in terms of the functions (5.4) on the combined phase space,

$$
\begin{aligned}
b(t)_0^{\pm}(\boldsymbol{x},\boldsymbol{p},\boldsymbol{n}) &= \tfrac{1}{2}\operatorname{tr}(\Delta_{1/2}(\boldsymbol{n})(V_\pm^* B(t)_0 V_\pm)(\boldsymbol{x},\boldsymbol{p}))\\
&= \tfrac{1}{2}\operatorname{tr}\big(D_\pm(\boldsymbol{x},\boldsymbol{p},t)\Delta_{1/2}(\boldsymbol{n})D_\pm^*(\boldsymbol{x},\boldsymbol{p},t)(V_\pm^* B_0 V_\pm)\big(\Phi_\pm^t(\boldsymbol{x},\boldsymbol{p})\big)\big)\\
&= b_0^{\pm}\big(\Phi_\pm^t(\boldsymbol{x},\boldsymbol{p}),\, R(D_\pm(\boldsymbol{x},\boldsymbol{p},t))\boldsymbol{n}\big)
\end{aligned}
$$

where in the last line the covariance (5.5) has been used. Hence, in leading semiclassical order the dynamics of an observable $\hat{B} \in \mathcal{O}_{\text{inv}}$ can be expressed in terms of the classical time evolutions

$$(\boldsymbol{x},\boldsymbol{p}) \mapsto \Phi_\pm^t(\boldsymbol{x},\boldsymbol{p}) \qquad \text{and} \qquad \boldsymbol{n} \mapsto \boldsymbol{n}_\pm(t) = R(D_\pm(\boldsymbol{x},\boldsymbol{p},t))\boldsymbol{n}. \tag{5.10}$$

The spin motion on the sphere thus emerging obeys the equation

$$\dot{\boldsymbol{n}}_\pm(t) = \boldsymbol{C}_\pm\big(\Phi_\pm^t(\boldsymbol{x},\boldsymbol{p})\big) \times \boldsymbol{n}_\pm(t) \qquad \boldsymbol{n}_\pm(0) = \boldsymbol{n} \tag{5.11}$$

that is implied by (5.9). These spin dynamics exactly coincide with the Thomas precession that was derived in a purely classical context [Tho27].

Both types of time evolutions in (5.10) can be combined to yield the dynamics

$$(\boldsymbol{x},\boldsymbol{p},\boldsymbol{n}) \mapsto Y_\pm^t(\boldsymbol{x},\boldsymbol{p},\boldsymbol{n}) := \big(\Phi_\pm^t(\boldsymbol{x},\boldsymbol{p}),\, R(D_\pm(\boldsymbol{x},\boldsymbol{p},t))\boldsymbol{n}\big) \tag{5.12}$$

on the phase space $\mathbb{R}^3 \times \mathbb{R}^3 \times \mathrm{S}^2$. The properties

$$Y_\pm^{t=0}(\boldsymbol{x},\boldsymbol{p},\boldsymbol{n}) = (\boldsymbol{x},\boldsymbol{p},\boldsymbol{n}) \qquad \text{and} \qquad Y_\pm^{t'+t}(\boldsymbol{x},\boldsymbol{p},\boldsymbol{n}) = Y_\pm^{t'}\big(Y_\pm^t(\boldsymbol{x},\boldsymbol{p},\boldsymbol{n})\big)$$

can easily be established, showing that (5.12) defines flows on the combined phase space. These flows are composed of the Hamiltonian flows $\Phi_\pm^t$ defined in (5.1) on the ordinary phase space $\mathbb{R}^3 \times \mathbb{R}^3$ and the spin dynamics (5.11) on S^2 that are driven by the Hamiltonian flows. Dynamical systems of this type are known as skew-product flows; see, e.g., [CFS82]. They leave the normalized measures

$$\mathrm{d}\ell_E^{\pm}(\boldsymbol{x},\boldsymbol{p})\,\mathrm{d}\boldsymbol{n} = \frac{1}{\operatorname{vol}\Omega_E^{\pm}}\delta(h_\pm(\boldsymbol{x},\boldsymbol{p}) - E)\,\mathrm{d}x\,\mathrm{d}p\,\mathrm{d}\boldsymbol{n}$$

on the combined phase space invariant that are products of Liouville measure $\mathrm{d}\ell_E^{\pm}(\boldsymbol{x},\boldsymbol{p})$ on $\Omega_E^{\pm}$ (microcanonical ensemble) and the normalized area measure $\mathrm{d}\boldsymbol{n}$ on S^2. We hence now conclude that the classical limit of the quantum dynamics generated by the Dirac–Hamiltonian (3.1) is given by the two skew-product flows (5.12) combining the Hamiltonian relativistic motion of (anti-) particles with the spin precession along the (anti-) particle trajectories.

6. Semiclassical behaviour of eigenspinors

In section 3 we saw that in general eigenspinors ψ_n of the Dirac–Hamiltonian (3.1) cannot uniquely be associated with either particles or anti-particles. For the purpose of semiclassical studies we therefore prefer to work with the normalized projected eigenspinors

$$\phi_n^{\pm} := \frac{\hat{P}^{\pm}\psi_n}{\|\hat{P}^{\pm}\psi_n\|}. \tag{6.1}$$

Due to the fact that the projectors almost commute with the Hamiltonian (3.8), the quantities (6.1) are almost eigenspinors (quasimodes) of both $\hat{H}$ and $\hat{H}\hat{P}^{\pm}$,

$$\big\|(\hat{H} - E_n)\phi_n^{\pm}\big\| = r_n^{\pm} \qquad \text{and} \qquad \big\|(\hat{H}\hat{P}^{\pm} - E_n)\phi_n^{\pm}\big\| = s_n^{\pm}$$

with error terms $r_n^{\pm}$ and $s_n^{\pm}$ given by

$$r_n^{\pm} = \frac{\|[\hat{H}, \hat{P}^{\pm}]\psi_n\|}{\|\hat{P}^{\pm}\psi_n\|} \qquad \text{and} \qquad s_n^{\pm} = \frac{\|[\hat{H}\hat{P}^{\pm}, \hat{P}^{\pm}]\psi_n\|}{\|\hat{P}^{\pm}\psi_n\|}.$$

Thus, if the norms $\|\hat{P}^{\pm}\psi_n\|$ of the projected eigenspinors are not too small, i.e. if $\|\hat{P}^{\pm}\psi_n\| \geqslant C\hbar^N$ holds for some $C > 0$ and $N < \infty$, the error terms $r_n^{\pm}$ and $s_n^{\pm}$ are of size $\hbar^{\infty}$.

This property implies that if the spectra of the operators $\hat{H}$ and $\hat{H}\hat{P}^{\pm}$ are discrete in the intervals $\left[E_n - r_n^{\pm}, E_n + r_n^{\pm}\right]$ and $\left[E_n - s_n^{\pm}, E_n + s_n^{\pm}\right]$, respectively, these operators each possess at least one eigenvalue in the respective interval; see, e.g., [Laz93]. For $\hat{H}$ the statement is trivial since E_n is known to be an eigenvalue, but regarding $\hat{H}\hat{P}^{\pm}$ it provides new insight. In particular, the mean spectral densities of the operators $\hat{H}\hat{P}^{\pm}$ are in general smaller than that of $\hat{H}$, see (6.2) below. Hence, the eigenvalues E_n of $\hat{H}$ must cluster in such a way that successive intervals $\left[E_n - r_n^{\pm}, E_n + r_n^{\pm}\right]$ overlap and therefore several such intervals share eigenvalues of $\hat{H}\hat{P}^{\pm}$. That way the separation of eigenvalues of $\hat{H}$ is linked with the norms of projected eigenspinors $\hat{P}^{\pm}\psi_n$. Suppose, e.g., all norms were bounded from below by $\|\hat{P}^{\pm}\psi_n\| \geqslant C\hbar^N$, such that $r_n^{\pm}, s_n^{\pm} = O(\hbar^{\infty})$, then sufficiently many eigenvalues E_n have to cluster on a scale $O(\hbar^{\infty})$. On the other hand, if the separations of neighbouring eigenvalues of $\hat{H}$ were known to be bounded from below by $\hbar^N$, a certain number of eigenspinor–projections would have to possess norms of size $\hbar^{\infty}$ in order to produce sufficiently large errors $r_n^{\pm}$.

More quantitative statements can be made on the ground of Weyl's law for the numbers $N_{E,\omega}$ and $N_{E,\omega}^{\pm}$ of eigenvalues the operators $\hat{H}$ and $\hat{H}\hat{P}^{\pm}$, respectively, possess in the interval $[E - \hbar\omega, E + \hbar\omega]$. Namely, as $\hbar \to 0$

$$N_{E,\omega} \sim \frac{2\omega}{\pi} \frac{\text{vol}\,\Omega_E^{+} + \text{vol}\,\Omega_E^{-}}{(2\pi\hbar)^2} \qquad N_{E,\omega}^{\pm} \sim \frac{2\omega}{\pi} \frac{\text{vol}\,\Omega_E^{\pm}}{(2\pi\hbar)^2}. \tag{6.2}$$

Thus, if at energy E both energy shells $\Omega_E^{\pm}$ in phase space have positive volumes, the ratios $N_{E,\omega}^{\pm}\big/N_{E,\omega}$ governing the previous discussion are semiclassically determined by the relative fraction of the volumes of the associated energy shells. Moreover, a version of Weyl's law that includes expectation values of operators (Szegö limit formula) yields [BG04]

$$N_{E,\omega}^{\pm} \sim \sum_{E-\hbar\omega \leqslant E_n \leqslant E+\hbar\omega} \|\hat{P}^{\pm}\psi_n\|^2. \tag{6.3}$$

This relation may suggest two (extreme) scenarios:

(i) Roughly $N_{E,\omega}^{\pm}$ of the projected eigenspinors $\hat{P}^{\pm}\psi_n$ are close to ψ_n and the remaining projections are semiclassically small.
(ii) The projections $\hat{P}^{\pm}\psi_n$ equidistribute on both energy shells in the sense that each $\|\hat{P}^{\pm}\psi_n\|^2$ is approximately $N_{E,\omega}^{\pm}\big/N_{E,\omega}$.

On the ground of the existing knowledge one cannot exclude either alternative, or a mixture of both. However, a comparison with symmetric versus asymmetric double-well potentials, where an eigenfunction either localizes in one well (asymmetric case, compare (i)), or has noticeable projections to both wells (symmetric case, compare (ii)), suggests that in generic cases, scenario (i) should be expected.

What is possible, though, is to estimate the number of projected eigenspinors with norms that are bounded from below,

$$N_{\delta}^{\pm} := \#\{n;\, E - \hbar\omega \leqslant E_n \leqslant E + \hbar\omega,\, \|\hat{P}^{\pm}\psi_n\|^2 \geqslant \delta\}.$$

From (6.2) and (6.3) it follows that

$$\lim_{\hbar\to 0}\frac{N_\delta^\pm}{N_{E,\omega}} \geqslant \frac{\operatorname{vol}\Omega_E^\pm}{\operatorname{vol}\Omega_E^+ + \operatorname{vol}\Omega_E^-} - \delta.$$

Therefore, if δ is sufficiently small (independent of $\hbar$) the right-hand side is positive and thus a finite portion of the projected eigenspinors has semiclassically non-vanishing norms. This observation allows us to take the associated normalized projected eigenspinors (6.1) into account for the following considerations.

We now explore the consequences an ergodic behaviour of the classical skew-product dynamics $Y_\pm^t$ exerts on the projected eigenspinors. In an analogous situation for Schrödinger–Hamiltonians the ergodicity of the associated Hamiltonian flow implies that the Wigner transforms of almost all eigenfunctions equidistribute on the corresponding energy shell. This result, known as quantum ergodicity, goes back to Shnirelman [Shn74] and has been fully proved in [Zel87, CdV85, HMR87]. In the case under study we now suppose that the energy E lies in an interval (E_-, E_+), in which the spectrum of the Dirac–Hamiltonian is discrete. Moreover, at least one of the classical energy shells Ω_E^+ and Ω_E^- shall be non-empty and the periodic orbits of the Hamiltonian flows $\Phi_\pm^t$ shall be of measure zero on $\Omega_E^\pm$. If then $Y_\pm^t$ is ergodic on $\Omega_E^\pm \times \mathrm{S}^2$, the time average of a classical observable of the type (5.4) equals its phase-space average,

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T b_0^\pm\big(Y_\pm^t(\boldsymbol{x},\boldsymbol{p},\boldsymbol{n})\big)\mathrm{d}t = \int_{\Omega_E^\pm}\int_{\mathrm{S}^2} b_0^\pm(\boldsymbol{x}',\boldsymbol{p}',\boldsymbol{n}')\,\mathrm{d}\ell_E^\pm(\boldsymbol{x}',\boldsymbol{p}')\,\mathrm{d}\boldsymbol{n}' =: M_E^\pm\big(b_0^\pm\big)$$

for almost all initial conditions $(\boldsymbol{x},\boldsymbol{p},\boldsymbol{n})$. In this setting the main result on quantum ergodicity of projected eigenspinors is (for a full proof see [BG04]) the following.

Theorem 6.1. *Under the conditions stated above, in particular if the skew-product flow $Y_\pm^t$ is ergodic on $\Omega_E^\pm \times \mathrm{S}^2$, in every sequence $\{\phi_n^\pm\}_{n\in\mathbb{N}}$ of normalized projected eigenspinors with associated eigenvalues $E_n \in [E-\hbar\omega, E+\hbar\omega]$ and $\|\hat{P}^\pm\psi_n\|^2 \geqslant \delta$ there exists a subsequence $\{\phi_{n_\alpha}^\pm\}_{\alpha\in\mathbb{N}}$ of density 1, i.e.*

$$\lim_{\hbar\to 0}\frac{\#\{\alpha;\ \|\hat{P}^\pm\psi_{n_\alpha}\|^2 \geqslant \delta\}}{\#\{n;\ \|\hat{P}^\pm\psi_n\|^2 \geqslant \delta\}} = 1$$

such that for every semiclassical observable $\hat{B} \in \mathcal{O}_{\mathrm{sc}}$

$$\lim_{\hbar\to 0}\big\langle\phi_{n_\alpha}^\pm, \hat{B}\phi_{n_\alpha}^\pm\big\rangle = M_E^\pm\big(b_0^\pm\big). \tag{6.4}$$

The density-1 subsequence $\{\phi_{n_\alpha}^\pm\}_{\alpha\in\mathbb{N}}$ can be chosen independent of the observable.

The statement of this theorem, which says that in the case of classical ergodicity quantum mechanical expectation values converge to a classical ergodic mean, can be rephrased in terms of more explicit phase-space lifts. To this end one first introduces the matrix-valued Wigner functions

$$W[\psi](\boldsymbol{x},\boldsymbol{p}) := \int_{\mathbb{R}^3} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{y}}\,\overline{\psi}\left(\boldsymbol{x}-\frac{1}{2}\boldsymbol{y}\right)\otimes\psi\left(\boldsymbol{x}+\frac{1}{2}\boldsymbol{y}\right)\mathrm{d}y$$

associated with any $\psi \in L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$. Following the prescription (5.4) this 4×4 matrix can be converted into scalar form through

$$w_\pm[\psi](\boldsymbol{x},\boldsymbol{p},\boldsymbol{n}) := \tfrac{1}{2}\operatorname{tr}(\Delta_{1/2}(\boldsymbol{n})(V_\pm^* W[\psi]V_\pm)(\boldsymbol{x},\boldsymbol{p})).$$

Due to the projections inherent in the expectation value on the left-hand side of (6.4) only one diagonal block of the observable contributes, so that this expectation value can be reformulated as

$$\begin{aligned}\langle\phi_{n_\alpha}^{\pm},\hat{B}\phi_{n_\alpha}^{\pm}\rangle &= \frac{1}{(2\pi\hbar)^3}\iint \mathrm{tr}\big(W\big[\phi_{n_\alpha}^{\pm}\big]P^{\pm}\#B\#P^{\pm}\big)(\boldsymbol{x},\boldsymbol{p})\,\mathrm{d}x\,\mathrm{d}p\\ &= \frac{1}{(2\pi\hbar)^3}\iint \mathrm{tr}\big(\big(V_{\pm}^{*}W\big[\phi_{n_\alpha}^{\pm}\big]V_{\pm}\big)(V_{\pm}^{*}B_0V_{\pm})(\boldsymbol{x},\boldsymbol{p})(1+O(\hbar))\big)\,\mathrm{d}x\,\mathrm{d}p\\ &= \frac{1}{(2\pi\hbar)^3}\iiint \big(w_{\pm}\big[\phi_{n_\alpha}^{\pm}\big](\boldsymbol{x},\boldsymbol{p},\boldsymbol{n})b_0^{\pm}(\boldsymbol{x},\boldsymbol{p},\boldsymbol{n})(1+O(\hbar))\big)\,\mathrm{d}x\,\mathrm{d}p\,\mathrm{d}\boldsymbol{n}.\end{aligned}$$

The principal result (6.4) of quantum ergodicity can hence be read as saying that

$$\lim_{\hbar\to 0}\frac{w_{\pm}\big[\phi_{n_\alpha}^{\pm}\big](\boldsymbol{x},\boldsymbol{p},\boldsymbol{n})}{(2\pi\hbar)^3} = \frac{1}{\mathrm{vol}\,\Omega_E^{\pm}}\delta(h_{\pm}(\boldsymbol{x},\boldsymbol{p})-E).$$

This relation has to be understood in a weak sense, i.e. after integration with a symbol $b_0^{\pm}(\boldsymbol{x},\boldsymbol{p},\boldsymbol{n})$. Hence, the scalar Wigner transforms of projected eigenspinors become semiclassically equidistributed on the associated phase space $\Omega_E^{\pm}\times \mathrm{S}^2$ once the classical time evolution $Y_{\pm}^{t}$ is ergodic on this space.

As the discussion at the beginning of this section shows, the difficulties with statements about genuine eigenspinors derive from the coexistence of the particle and anti-particle subspaces, and because interactions between these subspaces on a scale $\hbar^{\infty}$ cannot be controlled within the present setting. However, if one of the energy shells $\Omega_E^{\pm}$ was empty there is only one classical manifold onto which phase-space lifts of eigenspinors could condense, namely $\Omega_E^{\mp}\times \mathrm{S}^2$. In such a case, say when Ω_E^{-} is empty, the statement of theorem 6.1 applies to a density 1 subsequence $\{\psi_{n_\alpha}\}$ of eigenspinors themselves, such that

$$\lim_{\hbar\to 0}\big\langle\psi_{n_\alpha},\hat{P}^{+}\hat{B}\hat{P}^{+}\psi_{n_\alpha}\big\rangle = M_E^{\pm}\big(b_0^{\pm}\big) \qquad \text{and} \qquad \lim_{\hbar\to 0}\big\langle\psi_{n_\alpha},\hat{P}^{-}\hat{B}\hat{P}^{-}\psi_{n_\alpha}\big\rangle = 0. \tag{6.5}$$

A corresponding statement then holds for the associated scalar Wigner transforms $w_{\pm}\big[\psi_{n_\alpha}\big]$. It has been mentioned previously that the restriction of having only one non-empty energy shell at energy E requires potentials that do not vary too strongly; e.g., $\phi(\boldsymbol{x})$ must not vary as much as $2mc^2$. This condition is fulfilled in many physically relevant situations, in which (6.5) therefore applies if only the classical particle dynamics Y_{+}^{t} are ergodic.

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