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A semiclassical approach to the Dirac equation[1]

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Abstract

We derive a semiclassical time evolution kernel and a trace formula for the Dirac equation. The classical trajectories that enter the expressions are determined by the dynamics of relativistic point particles. We carefully investigate the transport of the spin degrees of freedom along the trajectories which can be understood geometrically as parallel transport in a vector bundle with SU(2) holonomy. Furthermore, we give an interpretation in terms of a classical spin vector that is transported along the trajectories and whose dynamics, dictated by the equation of Thomas precession, gives rise to dynamical and geometric phases every orbit is weighted by. We also present an analogous approach to the Pauli equation which we analyse in two different limits.

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1 Introduction

Most semiclassical approaches to the Dirac equation so far aimed at an extension of the WKB method, with the expectation that some kind of Bohr-Sommerfeld quantisation conditions would emerge in relativistic quantum mechanics. The earliest such approach is due to Pauli [1], who succeeded in showing that the phase of a WKB spinor is given by a solution of the Hamilton-Jacobi equation for relativistic point particles. But he could determine the amplitude of the semiclassical spinor only in some special cases. Although the programme mentioned above has been very successful in nonrelativistic quantum mechanics, where it leads to the so-called Einstein-Brillouin-Keller (EBK) quantisation [2], establishing semiclassical quantisation conditions in the case of the Dirac equation was found to be obstructed by the occurence of certain phases. Investigating multicomponent wave equations Yabana and Horiuchi [3] noticed that geometric phases play an important rôle in this context and have to be incorporated in appropriate quantisation conditions. Using path integrals instead of the WKB method, Kuratsuji and Iida [4, 5] realised that an inclusion of the geometric phases in the symplectic form on classical phase space offers a possibility to arrive at quantisation conditions. A general theory of semiclassical quantisation for multicomponent wave equations in arbitrary dimensions, which derive from classical Hamiltonian matrices with no globally degenerate eigenvalues, was developed by Littlejohn and Flynn [6, 7]. This method, however, does not apply to the Dirac Hamiltonian since the eigenvalues of the associated classical Hamiltonian matrix are twofold degenerate. Indeed, Emmrich and Weinstein [8] found that in the degenerate case integrability of the corresponding classical dynamics is not a sufficiently strong condition to allow for an extension of EBK quantisation to the case of multicomponent wave equations.

Moreover, even if successful, the procedure described above would not apply to systems whose classical limit is nonintegrable. In this paper we will therefore follow an alternative approach in that we investigate the semiclassical time evolution and then derive a semiclassical trace formula. This method is in the spirit of Gutzwiller's semiclassical treatment of the Schrödinger equation [9] (see also [10]), in which the quantum mechanical density of states is set into relation to a sum over the periodic orbits of the corresponding classical system. The geometric phases mentioned above also appear in our approach in that they represent the spin transport along classical orbits in the trace formula. The advantage of a trace formula approach is not only that it is applicable to both integrable and chaotic systems, but that it also provides the basis for efficient semiclassical quantisation conditions. In the context of quantum chaos extensive studies in this direction have been undertaken, see e. g. [11, 12]. Furthermore, semiclassical trace formulae are the primary tools for a semiclassical theory of spectral statistics, see e. g. [13, 14, 15, 16].

Before we go into more detail we want to take the opportunity to clarify our point of view regarding the semiclassical limit on which we base the following investigations. In general we will consider the mathematical limit $\hbar \to 0$, with the understanding that in a given physical situation an equivalent limit in terms of physical quantities such as controlable external parameters has to be taken. The effect of such a limit can then be expressed in terms of the spectrum of the Dirac Hamiltonian as follows. The l.h.s. of the trace formula that we are going to derive reads

$$\sum_n \varrho\left(\frac{E_n - E}{\hbar}\right) , \tag{1.1}$$

where the E_n's are the quantum mechanical eigenvalues, which depend on $\hbar$, and E denotes a variable parameter. The smooth test function ϱ decreases faster than any power for large arguments so that the main contribution to the sum comes from eigenvalues within an interval of length proportinal to $\hbar$,

$$E + \hbar\omega_1 < E_n < E + \hbar\omega_2 . \tag{1.2}$$

In the formal limit $\hbar \to 0$ the Weyl law forces the spectral density to increase in such a way that, although the length of the interval (1.2) shrinks to zero, infinitely many terms contribute to (1.1). In other words, the semiclassical limit corresponds to the limit of an increasing spectral density. The latter can possibly be achieved in a variety of different ways, which sometimes makes it necessary to vary several external parameters simultaneously. In case the limit $\hbar \to 0$ is accompanied by further limits, one then has to ensure that asymptotic expansions are uniform in the quantities that are involved in the further limits. Throughout this paper we will understand the semiclassical limit as being involved with the formal asymptotics as $\hbar \to 0$. In the last section, where we investigate the non-relativistic approximation of the results obtained for the Dirac equation, we briefly discuss an example with a second, simultaneous limit.

In the following sections we will develop the steps that are necessary to derive a trace formula for the Dirac equation in some detail. Basically we follow the method introduced by Gutzwiller [17, 18, 9] in the case of the Schrödinger equation. It turns out that regarding the translational degrees of freedom Gutzwiller's approach can indeed be taken over. The novel features that arise in the case of the Dirac equation derive from the spin degrees of freedom and their coupling to the translational dynamics. In section 2 we first fix our notation and recall the basic properties of the Dirac equation relevant for the following. Then we review the general rôle of periodic orbits in semiclassical trace formulae and introduce a regularisation procedure (cf. [19, 20]) which allows to obtain convergent trace formulae. We moreover recall how to cut off the essential spectrum of the Dirac Hamiltonian, which is present in most physically relevant situations and typically covers $(-\infty, -mc^2] \cup [mc^2, \infty)$.

Section 3 is devoted to the derivation of a semiclassical time evolution kernel in the spirit of the Van Vleck formula known for the respective kernel for the Schrödinger equation. In the present context we find it convenient to represent the time evolution kernel in terms of an oscillatory integral. This method was developed for the study of scalar wave equations in the context of microlocal analysis, see e. g. [21], and subsequently found application to the development of several trace formulae [22, 23, 19, 20]. In the case of the Schrödinger equation it leads to the same result as Gutzwiller's original derivation [17] which employed a stationary phase approximation of a Feynman path integral. The approach that we are going to follow is similar to the usual WKB method and results in equations that determine the coefficients of an $\hbar$-expansion of the time evolution kernel. The presence of spin is reflected in these equations through their matrix character. To lowest order one obtains as a condition for their solvability two Hamilton-Jacobi equations, which correspond to the classical dynamics of relativistic point particles with positive and negative kinetic energy, respectively. The condition that arises in next-to-leading order in $\hbar$ is usually called transport equation. The latter can be reduced to two differential equations for 2×2 matrices describing the transport of the spin degrees of freedom along particle orbits. The solutions of these spin transport equations as well as the solutions of the Hamilton-Jacobi equations finally determine the leading order of the semiclassical expansion for the time evolution operator. It is remarkable that the classical Hamiltonians do not include any term corresponding to forces acting on the magnetic moment of the spin. This fact was already realised by Pauli in his WKB treatment of the Dirac equation, see also a related discussion in [24]. For this reason Pauli's method was subsequently criticized by de Broglie [25], who argued that electromagnetic moments linked with the spin were classical quantities and therefore should be present in a semiclassical approximation. This objection was later clarified by Rubinow and Keller [26]. They pointed out that the moments of an electron are proportional to $\hbar$ so that in leading order as $\hbar \to 0$ the influence of spin on the trajectories vanishes. Furthermore, they showed how to obtain the equation describing the Thomas precession [27] of a classical spin, which is also known as the BMT-equation [28], from the transport equation. Since it only contains the ratio of the magnetic moment and the spin, $\hbar$ cancels from the equation of Thomas precession which therefore provides the correct description of a classical spin.

In section 4 we analyse the spin transport in more detail, where we mainly focus on two aspects. We first discuss the geometric terms that accompany semiclassical asymptotics of multicomponent wave equations as they follow from the transport equation. Their structure is of a similar form as discovered by Littlejohn and Flynn [7] in the case of wave equations with classical Hamiltonian matrices that have no (globally) degenerate eigenvalues. In particular, one contribution is identified as being of the same type as the Berry phase [29, 30, 31] appearing in adiabatic approximations. However, since in the case of the Dirac equation the eigenvalues of the classical Hamiltonian matrix are twofold degenerate, the U(1)-holonomy factors of Littlejohn and Flynn are replaced by corresponding SU(2) terms. Our results are found to be in accordance with the general discussion of the transport equation for multicomponent wave equations by Emmrich and Weinstein [8]. In addition, these authors revealed the global geometric meaning of all terms that contribute to the total holonomy following from the transport equation. As a second point we discuss how to express also the spin contributions to the semiclassical time evolution kernel in terms of classical quantities. To this end we introduce a classical spin vector $\vec{s}$ as an expectation value of a time dependent spin operator. It then follows from the spin transport equation that $\vec{s}$ has to fulfill the classical equation of Thomas precession. Thus, up to a phase factor the desired solution of the spin transport equation is determined by the classical spin precession along a given particle orbit. We also show that the additional phase factor is composed of a dynamical part associated with the energy of a classical magnetic moment in given electromagnetic fields, and a geometric part which is of the type discovered by Aharonov and Anandan [32].

In section 5 we derive the semiclassical trace formula for the Dirac equation, which is our central result, by Fourier transforming from the time domain to the energy domain and by subsequently taking the trace over spatial variables and matrix components. The periodic orbits that enter the trace formula are determined by the relativistic dynamics of classical point particles without internal degrees of freedom. The influence of the spin appears through two phase factors every periodic orbit is weighted by. One of these phases measures the change in the direction of the classical spin after this has been transported along a periodic orbit, whereas the second one contains the phase described above as being composed of a dynamical and a geometric part.

Finally, in section 6 we consider the nonrelativistic limit of the results obtained in the previous sections. It turns out that the leading order as $c \to \infty$ coincides with the result of an application of the above programme to the Pauli equation. This equation is also of independent interest because in applications it is often used to investigate spin-orbit coupling. Based on the method developed in [7], this important effect is e. g. treated semi-classically in [33, 34]. Frisk and Guhr [34] introduced a trace formula for a nonrelativistic Hamiltonian that describes spin-orbit coupling by modifying the Berry-Tabor trace formula [35] for classically integrable systems without spin. To be able to use the formalism of [7] they kept Bohr's magneton $\mu = \frac{e\hbar}{2mc}$ fixed as $\hbar \to 0$; otherwise the corresponding classical Hamiltonian matrix would have a twofold degenerate eigenvalue. This procedure is in contrast to our method which allows to treat $\hbar$ on the same footing in all terms. Fixing Bohr's magneton can be regarded as simultanously performing the limit $\hbar \to 0$ and the limit of an infinite coupling of spin to the translational degrees of freedom. In the semiclassical expressions the spin precession then decouples adiabatically from the translational motion. For the Pauli equation that describes a coupling of spin to an external magnetic field we compare two ways of performing the semiclassical limit: (i) $\hbar \to 0$ and (ii) $\hbar \to 0$, $|\vec{B}| \to 0$ with $\hbar\,|\vec{B}| = const$. In the first case the nonrelativisitic limit of the result for the Dirac equation emerges, where the geometric terms in the spin transport are SU(2)-holonomy factors. In the second case the adiabatic decoupling of the spin motion results in geometric terms that yield a U(1) holonomy such that the Berry phase of a precessing spin is recovered. Both results being different implies that the semiclassical limit $\hbar \to 0$ is not uniform in the magnetic field strength, a result that sheds some light on de Broglie's criticism of Pauli's approach.

2 Semiclassical asymptotics and classical trajectories

In this section we will present the basis for our subsequent discussion of semiclassical methods for the Dirac equation. In the following our focus will be on relativistic particles of charge e and mass m with spin 1/2 in external static electromagnetic fields. Thus the relevant Dirac equation reads

$$\mathrm{i}\hbar \frac{\partial \Psi}{\partial t}(\vec{x}, t) = \hat{H}_D \Psi(\vec{x}, t) \;, \tag{2.1}$$

with the quantum Hamiltonian

$$\hat{H}_D := c\vec{\alpha}\left(\frac{\hbar}{\mathrm{i}}\vec{\nabla}_{\vec{x}} - \frac{e}{c}\vec{A}(\vec{x})\right) + \beta mc^2 + e\,\varphi(\vec{x})\ , \tag{2.2}$$

which is a matrix-valued differential operator of first order. Here φ and $\vec{A}$ denote the electromagnetic potentials such that the corresponding fields are given by $\vec{E}(\vec{x}) = -\vec{\nabla}_{\vec{x}}\varphi(\vec{x})$ and $\vec{B}(\vec{x}) = \vec{\nabla}_{\vec{x}} \times \vec{A}(\vec{x})$. The Dirac algebra is realised by the 4×4 matrices

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}\ , \tag{2.3}$$

where $\vec{\sigma}$ denotes the vector of Pauli matrices, and $\mathbb{1}_k$ is the $k \times k$ unit matrix; see [36] for further details. The Hamiltonian (2.2) can be realised as

$$\hat{H}_D = H_D\left(\frac{\hbar}{\mathrm{i}}\vec{\nabla}_{\vec{x}}, \vec{x}\right)\ , \tag{2.4}$$

where

$$H_D\left(\vec{p}, \vec{x}\right) := c\vec{\alpha}\left(\vec{p} - \frac{e}{c}\vec{A}(\vec{x})\right) + \beta mc^2 + e\,\varphi(\vec{x}) \tag{2.5}$$

is the symbol matrix, in the sense of Weyl quantisation, of the operator $\hat{H}_D$ (see e. g. [37]). In case the potentials φ and $\vec{A}$ satisfy suitable regularity conditions, the Dirac Hamiltonian $\hat{H}_D$, when defined on the domain $C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^4$ in the Hilbert space $\mathcal{H} := L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$, is essentially self-adjoint; see e. g. [38, 39]. In the following we will always deal with its self-adjoint extension which we also denote by $\hat{H}_D$.

Solutions $\Psi(\vec{x}, t)$ of the Dirac equation (2.1), with initial conditions $\Psi(\vec{x}, 0) = \Psi_0(\vec{x}) \in \mathcal{H}$, are obtained as $\hat{U}(t)\Psi_0 = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_D t}\Psi_0$. The time evolution operator $\hat{U}(t)$ can then be represented by its Schwartz kernel $K(\vec{x}, \vec{y}, t)$, so that

$$\Psi(\vec{x}, t) = \int_{\mathbb{R}^3} K(\vec{x}, \vec{y}, t)\, \Psi_0(\vec{y})\ \mathrm{d}^3 y\ . \tag{2.6}$$

This matrix-valued kernel is obviously required to solve the Dirac equation, with initial condition

$$\lim_{t \to 0^+} K(\vec{x}, \vec{y}, t) = \mathbb{1}_4\, \delta(\vec{x} - \vec{y})\ . \tag{2.7}$$

Our first major goal, to be dealt with in the next section, will be to derive a semiclassical representation of the time evolution kernel $K(\vec{x}, \vec{y}, t)$ in the spirit of the Van Vleck formula for the respective kernel of the Schrödinger equation. In the latter case such a representation is usually derived from a Feynman path integral, to which the method of stationary phase is applied [17]. Here we prefer an alternative semiclassical approach that makes use of a representation of the kernel in terms of an oscillatory integral. This method has previously also proven useful in the case of the Schrödinger equation, see e. g. [40, 16], in which it served as a basis for a mathematically rigorous proof [19, 20] of the Gutzwiller trace formula [9, 10].

We therefore now introduce the matrix-valued oscillatory integral

$$K(\vec{x},\vec{y},t) = \frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^3}\left[a_\hbar^+(\vec{x},\vec{y},t;\vec{\xi})\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi^+(\vec{x},\vec{y},t;\vec{\xi})} + a_\hbar^-(\vec{x},\vec{y},t;\vec{\xi})\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi^-(\vec{x},\vec{y},t;\vec{\xi})}\right]\,\mathrm{d}^3\xi\ , \tag{2.8}$$

where $\phi^\pm$ are real-valued smooth phase functions that are independent of $\hbar$, and $a_\hbar^\pm$ are 4×4 matrices with semiclassical expansions

$$a_\hbar^\pm(\vec{x},\vec{y},t;\vec{\xi}) = \sum_{k=0}^{\infty}\left(\frac{\hbar}{\mathrm{i}}\right)^k a_k^\pm(\vec{x},\vec{y},t;\vec{\xi}) + O(\hbar^\infty)\ . \tag{2.9}$$

According to the general theory of Schwartz kernels, $K(\vec{x},\vec{y},t)$ is a distribution kernel so that the integral (2.8) has to be interpreted in a distributional sense, see e. g. [40] for details in the scalar case. In order to account for the initial condition (2.7) one chooses

$$\phi^\pm(\vec{x},\vec{y},0;\vec{\xi}) = (\vec{x}-\vec{y})\vec{\xi}\ , \tag{2.10}$$

and

$$a_k^+(\vec{x},\vec{y},0;\vec{\xi}) + a_k^-(\vec{x},\vec{y},0;\vec{\xi}) = \begin{cases}\mathbb{1}_4 & \text{if } k=0\ ,\\ 0 & \text{if } k\geq 1\ .\end{cases} \tag{2.11}$$

Since the kernel (2.8) has to solve the Dirac equation, one obtains conditions for the phases $\phi^\pm$ and the coefficients $a_k^\pm$ appearing in the matrix-valued amplitudes $a_\hbar^\pm$. A detailed discussion of these equations will be postponed to the next section. Here we only remark that the phase functions have to satisfy the Hamilton-Jacobi equations

$$H^\pm\left(\vec{\nabla}_{\vec{x}}\phi^\pm(\vec{x},\vec{y},t;\vec{\xi}),\vec{x}\right) + \frac{\partial\phi^\pm}{\partial t}(\vec{x},\vec{y},t;\vec{\xi}) = 0\ , \tag{2.12}$$

with the classical Hamiltonians

$$H^\pm(\vec{p},\vec{x}) = e\varphi(\vec{x}) \pm \sqrt{c^2\left(\vec{p}-\frac{e}{c}\vec{A}(\vec{x})\right)^2 + m^2c^4} \tag{2.13}$$

of relativistic particles with positive (+) and negative (−) kinetic energies, respectively. As can readily be verified, the functions $H^\pm(\vec{p},\vec{x})$ are the two, twofold degenerate, eigenvalues of the symbol matrix (2.5). A posteriori, the occurrence of two Hamilton-Jacobi equations (2.12) justifies the choice (2.8) of the oscillatory integral with two additive contributions.

Due to the form (2.12) of the Hamilton-Jacobi equations and the initial conditions (2.10), the variable $\vec{y}$ can be separated according to

$$\phi^\pm(\vec{x},\vec{y},t;\vec{\xi}) = S^\pm(\vec{x},\vec{\xi},t) - \vec{y}\vec{\xi}\ , \tag{2.14}$$

so that the functions $S^{\pm}(\vec{x},\vec{\xi},t)$ also solve the Hamilton-Jacobi equations (2.12), but with initial conditions $S^{\pm}(\vec{x},\vec{\xi},0)=\vec{x}\vec{\xi}$. From general Hamilton-Jacobi theory, see e. g. [41, 40], it is known that therefore $S^{\pm}(\vec{x},\vec{\xi},t)$ are generating functions for canonical transformations $(\vec{p},\vec{x})\mapsto(\vec{\xi},\vec{z})$. For ease of notation we restrict the following discussion to the index $+$. Then $(\vec{p},\vec{x})$ are the end points of the solution $(\vec{P}(t'),\vec{X}(t'))$ of Hamilton's equations of motion, generated by the Hamiltonian H^{+}, with initial condition $(\vec{\xi},\vec{z})$. This means that

$$(\vec{P}(0),\vec{X}(0))=(\vec{\xi},\vec{z}) \quad \text{and} \quad (\vec{P}(t),\vec{X}(t))=(\vec{p},\vec{x})\ . \tag{2.15}$$

In order to explicitly incorporate the initial conditions we will also use the notation

$$\vec{P}(t')=\vec{P}(t';\vec{\xi},\vec{z}) \quad \text{and} \quad \vec{X}(t')=\vec{X}(t';\vec{\xi},\vec{z}) \quad \text{for} \quad 0\le t'\le t\ . \tag{2.16}$$

The fact that $S^{+}(\vec{x},\vec{\xi},t)$ is a generating function for the associated canonical transformation moreover implies the relations

$$\vec{p}=\vec{\nabla}_{\vec{x}}S^{+}(\vec{x},\vec{\xi},t) \quad \text{and} \quad \vec{z}=\vec{\nabla}_{\vec{\xi}}S^{+}(\vec{x},\vec{\xi},t)\ . \tag{2.17}$$

For sufficiently small times, $|t|<t_c$, the Hamilton-Jacobi equations (2.12) are known to possess unique solutions $S^{\pm}(\vec{x},\vec{\xi},t)$, see e. g. [40]. However, it is well known that at some critical time t_c a caustic may arise so that for $|t|\ge t_c$ the solutions of the Hamilton-Jacobi equations are no longer unique. The representation (2.8) of the time evolution kernel for $|t|\ge t_c$ can then only be a local one. A global object has to be constructed by gluing appropriate local representations together. This procedure requires consistency conditions, which are reflected by the presence of Morse indices in the final semiclassical expression to be derived in section 3. For the Schrödinger equation this was already noticed by Gutzwiller [17]. A mathematically rigorous construction employing the Maslov bundle can be found in [19]. For simplicity, we will neglect this problem below in that we continue to work with (2.8) and only in the end introduce the appropriate phase factors.

Since the principal applications of semiclassical trace formulae deal with eigenvalues of quantum Hamiltonians, in particular with their semiclassical determination and their statistical properties, respectively, one would like to isolate the point spectrum of $\hat{H}_D$ from its essential spectrum. In case the potentials φ and $\vec{A}$ vanish towards spatial infinity, or under suitably weakened conditions, the essential spectrum is known to be given by $\mathbb{R}\backslash(-mc^2,mc^2)$, see e. g. [38, 39], so that for the following we assume $\hat{H}_D$ to have, possibly infinitely many, eigenvalues of finite multiplicities in the interval $(-mc^2,mc^2)$. Given any interval $I=(E_a,E_b)$ that contains only isolated eigenvalues, we introduce a smooth function $\chi(E)$ that is supported in I, i. e., it vanishes outside of I, such that $\chi(E)=1$ on a suitably large subinterval. In particular, if there is no accumulation of eigenvalues at E_a or E_b, one can achieve that $\chi(E_n)=1$ for all eigenvalues E_n of $\hat{H}_D$. Otherwise, as e. g. for the Dirac Hamiltonian of the hydrogen atom, one can enlarge the support of χ arbitrarily towards $\pm mc^2$ so that arbitrarily many eigenvalues can be taken into account. Then the operator $\chi(\hat{H}_D)$, defined by the functional calculus given by the spectral theorem, is bounded and self-adjoint; see e. g. [40] for the scalar case. This operator has a purely discrete spectrum with eigenvalues $\chi(E_n)$. Therefore the Schwartz kernel $K_\chi(\vec{x},\vec{y},t)$ of the truncated time evolution operator $\hat{U}_\chi(t) := \chi(\hat{H}_D)\,\hat{U}(t)$ has a spectral representation

$$K_\chi(\vec{x},\vec{y},t) = \sum_n \chi(E_n)\,\Psi_n(\vec{x})\Psi_n^\dagger(\vec{y})\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_n t} \tag{2.18}$$

in terms of the orthonormal eigenspinors Ψ_n of $\hat{H}_D$, where $\Psi_n^\dagger$ denotes the hermitian adjoint of Ψ_n. According to the definition of the truncated time evolution operator, which implies that

$$\left(\hat{U}_\chi(t)\Psi_0\right)(\vec{x}) = \chi(\hat{H}_D)\,\Psi(\vec{x},t)\ , \tag{2.19}$$

the truncated kernel is obtained from the non-truncated one as

$$\begin{aligned} K_\chi(\vec{x},\vec{y},t) &= \chi(\hat{H}_D)\,K(\vec{x},\vec{y},t) \\ &= \frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^3}\chi(\hat{H}_D)\left[a_\hbar^+(\vec{x},\vec{y},t;\vec{\xi})\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi^+(\vec{x},\vec{y},t;\vec{\xi})} + a_\hbar^-(\vec{x},\vec{y},t;\vec{\xi})\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi^-(\vec{x},\vec{y},t;\vec{\xi})}\right]\,\mathrm{d}^3\xi\ ; \end{aligned} \tag{2.20}$$

here $\chi(\hat{H}_D)$ always acts on functions of $\vec{x}$. In the framework of Weyl calculus one can identify the symbol of the operator $\chi(\hat{H}_D)$ to possess a semiclassical expansion with principal symbol (leading term) $\chi(H_D(\vec{p},\vec{x}))$, see [40]. Thus, an explicit calculation yields that

$$\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\phi(\vec{x})}\left(\chi(\hat{H}_D)\,a\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi}\right)(\vec{x}) = \chi\left(H_D(\vec{\nabla}_{\vec{x}}\phi(\vec{x}),\vec{x})\right)\,a(\vec{x}) + O(\hbar)\ , \tag{2.21}$$

for any sufficiently regular matrix-valued function a and real-valued function ϕ. This calculation is closely parallel to the respective result in the scalar case, which can be found in [21]. Notice that in [21] a different quantisation is used which, however, yields to lowest semiclassical order the same result as Weyl quantisation. Thus, to leading order in $\hbar$, the truncated time evolution kernel reads

$$\begin{aligned} K_\chi(\vec{x},\vec{y},t) = \frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^3}\Big[&\chi(H_D(\vec{\nabla}_{\vec{x}}\phi^+,\vec{x}))\,a_0^+\,(1+O(\hbar))\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi^+} \\ &+\chi(H_D(\vec{\nabla}_{\vec{x}}\phi^-,\vec{x}))\,a_0^-\,(1+O(\hbar))\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi^-}\Big]\,\mathrm{d}^3\xi\ . \end{aligned} \tag{2.22}$$

In order to prepare for the semiclassical trace formula to be dealt with in section 5 we now introduce a regularisation of the truncated time evolution operator. To this end consider a smooth test function $\varrho \in C^\infty(\mathbb{R})$ such that its Fourier transform

$$\tilde{\varrho}(t) := \int_{-\infty}^{+\infty}\varrho(E)\,\mathrm{e}^{iEt}\,\mathrm{d}E \tag{2.23}$$

is smooth and compactly supported. Then in particular, both ϱ and $\tilde{\varrho}$ are test functions from the Schwartz space $\mathcal{S}(\mathbb{R})$. We now define the (bounded) operator

$$\hat{U}_\chi[\tilde{\varrho}] := \frac{1}{2\pi}\int_{-\infty}^{+\infty}\tilde{\varrho}(t)\,\hat{U}_\chi(t)\,\mathrm{d}t\ , \tag{2.24}$$

whose trace can be calculated with the spectral representation (2.18) of the truncated time evolution kernel as

$$\mathrm{Tr}\,\hat{U}_\chi[\tilde{\varrho}] = \frac{1}{2\pi}\int_{\mathbb{R}^3}\int_{-\infty}^{+\infty} \tilde{\varrho}(t)\ \mathrm{tr}\,K_\chi(\vec{x},\vec{x},t)\ \mathrm{d}t\,\mathrm{d}^3x = \sum_n \chi(E_n)\,\varrho\left(\frac{E_n}{\hbar}\right)\ . \tag{2.25}$$

Here Tr means the operator trace on $L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$, which includes a trace over the matrix components; the latter is denoted by tr. The linear map $\tilde{\varrho}\mapsto \mathrm{Tr}\,\hat{U}_\chi[\tilde{\varrho}]$ defines a tempered distribution, denoted by $\mathrm{Tr}\,\hat{U}_\chi[\cdot]\in\mathcal{S}'(\mathbb{R})$, if the sum on the r.h.s. of (2.25) converges absolutely. To this end one requires that

$$\left|\chi(E_n)\,\varrho\left(\frac{E_n}{\hbar}\right)\right| = O\left(\frac{1}{n^{1+\varepsilon}}\right)\ ,\quad \varepsilon>0\ ,\quad n\to\infty\ . \tag{2.26}$$

The simplest case of finitely many eigenvalues in the support of χ obviously poses no problem. If, however, eigenvalues accumulate at some $E_{acc}\in[-mc^2,mc^2]$, the truncation χ has to be chosen such that $\chi(E_{acc})=0$ and, moreover, $\chi(E)$ vanishes sufficiently fast as $E\to E_{acc}$ in order to fulfill (2.26). We now evaluate the distribution $\mathrm{Tr}\,\hat{U}_\chi[\cdot]$ on the test function $\tilde{\varrho}(t)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}Et}$ and thus obtain the relation

$$\sum_n \chi(E_n)\,\varrho\left(\frac{E_n-E}{\hbar}\right) = \frac{1}{2\pi}\int_{\mathbb{R}^3}\int_{-\infty}^{+\infty} \tilde{\varrho}(t)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}Et}\ \mathrm{tr}\,K_\chi(\vec{x},\vec{x},t)\ \mathrm{d}t\,\mathrm{d}^3x\ . \tag{2.27}$$

The semiclassical trace formula we are aiming at results, if for the truncated time evolution kernel in (2.27) one introduces a semiclassical representation and calculates the integrals with the method of stationary phase. The details of this procedure will be carried out in section 5. Here we only remark that upon introducing the representation (2.22) for the kernel, in leading semiclassical order one has to compute the integrals

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{-\infty}^{+\infty} \tilde{\varrho}(t)\,\chi(H_D(\vec{\nabla}_{\vec{x}}\phi^\pm(\vec{x},\vec{x},t;\vec{\xi}),\vec{x}))\,a_0^\pm(\vec{x},\vec{x},t;\vec{\xi})\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}[\phi^\pm(\vec{x},\vec{x},t;\vec{\xi})+Et]}\ \mathrm{d}t\,\mathrm{d}^3x\,\mathrm{d}^3\xi\ . \tag{2.28}$$

According to the method of stationary phase, see e. g. [40, 21], all contributions to (2.28) that exceed $O(\hbar^\infty)$ as $\hbar\to 0$ are determined by the stationary points, in the variables $(\vec{\xi},\vec{x},t)$, of the phase $\phi^\pm(\vec{x},\vec{x},t;\vec{\xi})+Et$. These stationary points are solutions of the equations

$$\begin{aligned}\left[\vec{\nabla}_{\vec{x}}\phi^\pm(\vec{x},\vec{y},t;\vec{\xi})+\vec{\nabla}_{\vec{y}}\phi^\pm(\vec{x},\vec{y},t;\vec{\xi})\right]_{\vec{y}=\vec{x}} &= 0\ ,\\ \frac{\partial\phi^\pm}{\partial t}(\vec{x},\vec{x},t;\vec{\xi})+E &= 0\ ,\\ \vec{\nabla}_{\vec{\xi}}\phi^\pm(\vec{x},\vec{x},t;\vec{\xi}) &= 0\ .\end{aligned} \tag{2.29}$$

If one now recalls the connection (2.14) of the phase $\phi^\pm$ to the generating function $S^\pm$, one obtains the equivalent conditions

$$\vec{\nabla}_{\vec{\xi}} S^\pm(\vec{x},\vec{\xi},t) = \vec{x} \quad , \quad \vec{\nabla}_{\vec{x}} S^\pm(\vec{x},\vec{\xi},t) = \vec{\xi} \quad , \quad \frac{\partial S^\pm}{\partial t}(\vec{x},\vec{\xi},t) = -E \ , \tag{2.30}$$

to be fulfilled by stationary points $(\vec{\xi},\vec{x},t)$. A comparison with the relations (2.17) now yields the conditions $\vec{\xi} = \vec{p}$ and $\vec{x} = \vec{z}$, so that the stationary points determine periodic solutions, with energy E, of Hamilton's equations of motion generated by the Hamiltonians (2.13). We denote these periodic orbits by $\gamma_p^\pm$. Their periods, given by the t-components of the corresponding stationary points, are called $T_{\gamma_p^\pm}$. Notice that our requirement on the test function $\tilde{\varrho}$ to have compact support implies that only periodic orbits up to some finite period, $|T_{\gamma_p^\pm}| \leq T_{max}$, contribute. However, since the support of $\tilde{\varrho}$ can be made arbitrarily large one can manage to include as many periodic orbits as desired. As our first observation on the way towards a semiclassical trace formula we thus now conclude that, apart from terms of $O(\hbar^\infty)$, in the semiclassical limit $\hbar \to 0$ all contributions to the l.h.s. of (2.27) are due to classical periodic orbits of energy E of relativistic point particles.

A further observation can be made with (2.28) if the set of stationary points $(\vec{\xi},\vec{x},t)$ divides into a sequence M_k, $k \in \mathbb{N}_0$, of m_k-dimensional smooth submanifolds of $\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}$ such that the phase $S^\pm(\vec{x},\vec{\xi},t) - \vec{x}\vec{\xi} + Et$ is non-degenerate transversal to the manifolds M_k. The latter condition means that the matrix of second derivatives of the phase with respect to $(\vec{\xi},\vec{x},t)$ has constant rank $7 - m_k$ when restricted to M_k. The flow generated by $H^\pm$ is then called clean, see [19, 20] for further details. In this situation the set of periods is known to be discrete in $\mathbb{R}$ [42]. Thus the periods cannot accumulate at some finite value T. Under these conditions the method of stationary phase implies that each manifold M_k yields a contribution

$$\hbar^{\frac{1-m_k}{2}} \mathcal{A}_{M_k}(\hbar)\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar} S_{M_k}} + O(\hbar^\infty) \ , \quad \text{with} \quad \mathcal{A}_{M_k}(\hbar) = \sum_{j=0}^{\infty} \hbar^j \mathcal{A}_{M_k,j} \ , \tag{2.31}$$

to (2.27). Here S_{M_k} is the action of any periodic orbit $\gamma_p^\pm$ contained in M_k, which can be computed as the integral of the canonical one-form $\vec{p}\,\mathrm{d}\vec{x}$ along any closed path on M_k. The coefficients $\mathcal{A}_{M_k,j}$ are independent of $\hbar$ and arise in the method of stationary phase as certain integrals over M_k. In the case of an isolated periodic orbit $\gamma_p^\pm$ the manifold M_k is given by the points on the primitive periodic orbit associated with $\gamma_p^\pm$, and thus $m_k = 1$. If the phase is non-degenerate transversal to an isolated periodic orbit, the latter is called non-degenerate. For this situation we will explicitly calculate $\mathcal{A}_{M_k,0}$ in section 5. Another case that can be dealt with explicitly concerns the hypersurfaces

$$\Omega_E^\pm := \big\{(\vec{p},\vec{x});\ H^\pm(\vec{p},\vec{x}) = E\big\} \tag{2.32}$$

of constant energy E in phase space. The points $(\vec{p},\vec{x}) \in \Omega_E^\pm$ are obviously periodic under the flows generated by $H^\pm$, with trivial period $T_0 = 0$. Since according to the above non-degeneracy condition we assume that $M_0^\pm = \Omega_E^\pm \times \{0\}$ are (five dimensional) smooth manifolds, E is required to be a regular value for the respective flows. Moreover, the associated leading terms in (2.31) are of the order $\hbar^{-2}$. The explicit calculation of $\mathcal{A}_{M_0^\pm,0}$ will also be performed in section 5. As a final remark let us mention that in case the dynamics generated by $H^\pm$ are integrable, phase space foliates into three dimensional invariant tori such that the respective manifolds M_k are given by the rational ones among these tori. Thus $m_k = 3$ so that the leading terms in (2.31) are of the order $\hbar^{-1}$.

3 Semiclassical time evolution

In this section we will determine semiclassical representations for the time evolution kernel $K(\vec{x},\vec{y},t)$ and its truncated version $K_\chi(\vec{x},\vec{y},t)$, respectively. In a first step we derive necessary conditions that must be imposed on the matrix-valued amplitudes $a_\hbar^\pm$ and on the real-valued phases $\phi^\pm$ in order that the oscillatory integral (2.8) be a possible ansatz for the time evolution kernel. In a second step we then employ the method of stationary phase to (2.8), and from the result we obtain a semiclassical expression in the spirit of the Van Vleck formula for the respective kernel of the Schrödinger equation.

The requirement that (2.8), together with the expansion (2.9), be a semiclassical representation of the kernel $K(\vec{x},\vec{y},t)$ to all orders in $\hbar$ means that the oscillatory integral shall fulfill the Dirac equation (2.1) up to terms $O(\hbar^\infty)$. We therefore act with $\hat{H}_D - \mathrm{i}\hbar\frac{\partial}{\partial t}$ on (2.8) after having introduced the expansion (2.9), and then group terms of like orders in $\hbar$. The phases $\phi^\pm$ and coefficients $a_k^\pm$ now have to satisfy equations that result from demanding that all coefficients of powers $\hbar^k$, $k = 0, 1, 2, \ldots$, vanish. To lowest order ($k = 0$) one thus obtains the equation

$$\begin{aligned} &\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi^+(\vec{x},\vec{y},t;\vec{\xi})}\left[H_D\left(\vec{\nabla}_{\vec{x}}\phi^+(\vec{x},\vec{y},t;\vec{\xi}),\vec{x}\right) + \frac{\partial\phi^+}{\partial t}(\vec{x},\vec{y},t;\vec{\xi})\right]a_0^+(\vec{x},\vec{y},t;\vec{\xi}) \\ &\quad + \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi^-(\vec{x},\vec{y},t;\vec{\xi})}\left[H_D\left(\vec{\nabla}_{\vec{x}}\phi^-(\vec{x},\vec{y},t;\vec{\xi}),\vec{x}\right) + \frac{\partial\phi^-}{\partial t}(\vec{x},\vec{y},t;\vec{\xi})\right]a_0^-(\vec{x},\vec{y},t;\vec{\xi}) = 0\ , \end{aligned} \tag{3.1}$$

in which $H_D(\vec{p},\vec{x})$ denotes the symbol matrix (2.5) of the quantum Hamiltonian $\hat{H}_D$. For the following it turns out to be convenient to demand an individual vanishing of the terms with index $+$ and $-$, respectively. Since the two twofold degenerate eigenvalues of the hermitian 4×4 symbol matrix $H_D(\vec{p},\vec{x})$ are given by $H^\pm(\vec{p},\vec{x})$, see (2.13), the condition (3.1) can be fulfilled as soon as the matrices $a_0^\pm$ are suitably composed of eigenvectors of $H_D(\vec{\nabla}_{\vec{x}}\phi^\pm,\vec{x})$. Upon diagonalising the symbol matrix $H_D(\vec{p},\vec{x})$ one obtains an orthonormal basis for $\mathbb{C}^4$ (endowed with the canonical scalar product) that consists of eigenvectors $\{e_1(\vec{p},\vec{x}), e_2(\vec{p},\vec{x})\}$ with eigenvalue $H^+(\vec{p},\vec{x})$, and eigenvectors $\{f_1(\vec{p},\vec{x}), f_2(\vec{p},\vec{x})\}$ with eigenvalue $H^-(\vec{p},\vec{x})$. We now define the 4×2 matrices $V(\vec{p},\vec{x})$ and $W(\vec{p},\vec{x})$ whose two coloumns are given by the vectors $e_1(\vec{p},\vec{x}), e_2(\vec{p},\vec{x})$ and $f_1(\vec{p},\vec{x}), f_2(\vec{p},\vec{x})$, respectively. In explicit terms these matrices read

$$
\begin{aligned}
V(\vec{p},\vec{x}) &= \frac{1}{\sqrt{2\varepsilon(\vec{p},\vec{x})[\varepsilon(\vec{p},\vec{x})+mc^2]}}\begin{pmatrix}[\varepsilon(\vec{p},\vec{x})+mc^2]\,\mathbb{1}_2\\ [c\vec{p}-e\vec{A}(\vec{x})]\,\vec{\sigma}\end{pmatrix}\ ,\\
W(\vec{p},\vec{x}) &= \frac{1}{\sqrt{2\varepsilon(\vec{p},\vec{x})[\varepsilon(\vec{p},\vec{x})+mc^2]}}\begin{pmatrix}[c\vec{p}-e\vec{A}(\vec{x})]\,\vec{\sigma}\\ -[\varepsilon(\vec{p},\vec{x})+mc^2]\,\mathbb{1}_2\end{pmatrix}\ ,
\end{aligned}
\tag{3.2}
$$

where

$$
\varepsilon(\vec{p},\vec{x}) := \sqrt{\left(c\,\vec{p}-e\,\vec{A}(\vec{x})\right)^2+m^2c^4} = H^+(\vec{p},\vec{x})-e\varphi(\vec{x})\ . \tag{3.3}
$$

Since the eigenvectors $\{e_1,e_2,f_1,f_2\}$ are chosen to be orthonormal and form a basis for $\mathbb{C}^4$, one obtains the relations

$$
V^\dagger V = \mathbb{1}_2\ ,\quad W^\dagger W = \mathbb{1}_2\ ,\quad V\,V^\dagger + W\,W^\dagger = \mathbb{1}_4\ . \tag{3.4}
$$

Moreover, the projectors $P_\pm(\vec{p},\vec{x})$ onto the eigenspaces corresponding to the eigenvalues $H^\pm(\vec{p},\vec{x})$, respectively, are given by $P_+ = V\,V^\dagger$ and $P_- = W\,W^\dagger$.

Following (2.14), we now choose the generating functions $S^\pm$ to replace the phase functions $\phi^\pm$. If one then introduces suitable 2×4 matrices $\widetilde{V}$ and $\widetilde{W}$,

$$
\begin{aligned}
a_0^+(\vec{x},\vec{y},t;\vec{\xi}) &= V\left(\vec{\nabla}_{\vec{x}}S^+(\vec{x},\vec{\xi},t),\vec{x}\right)\,\widetilde{V}(\vec{x},\vec{\xi},t)\ ,\\
a_0^-(\vec{x},\vec{y},t;\vec{\xi}) &= W\left(\vec{\nabla}_{\vec{x}}S^-(\vec{x},\vec{\xi},t),\vec{x}\right)\,\widetilde{W}(\vec{x},\vec{\xi},t)\ ,
\end{aligned}
\tag{3.5}
$$

the condition (3.1) is fulfilled as soon as $S^\pm$, and hence also the phases $\phi^\pm$, satisfy the Hamilton-Jacobi equations

$$
H^\pm\left(\vec{\nabla}_{\vec{x}}S^\pm(\vec{x},\vec{\xi},t),\vec{x}\right)+\frac{\partial S^\pm}{\partial t}(\vec{x},\vec{\xi},t) = 0\ . \tag{3.6}
$$

In the definition of the matrices $\widetilde{V}$ and $\widetilde{W}$ we anticipated the fact that the coefficients $a_k^\pm$ are independent of $\vec{y}$, see the discussion below (3.8). At the moment an explicit expression for $\widetilde{V}$ and $\widetilde{W}$ is not needed. After having applied the method of stationary phase to (2.8) we will specify them further. Here we only remark that in order to fulfill the initial condition (2.11) we demand that

$$
\widetilde{V}(\vec{x},\vec{\xi},0) = V^\dagger(\vec{\xi},\vec{x})\quad\text{and}\quad \widetilde{W}(\vec{x},\vec{\xi},0) = W^\dagger(\vec{\xi},\vec{x})\ , \tag{3.7}
$$

so that $a_0^\pm(\vec{x},\vec{y},0;\vec{\xi}) = P_\pm(\vec{\xi},\vec{x})$. In conclusion, the condition (3.1) to lowest order in $\hbar$ requires the phases $\phi^\pm$ to solve the Hamilton-Jacobi equations (2.12). Due to the initial condition (2.10) these functions are therefore now completely fixed.

Our next goal is to determine the leading contributions $a_0^\pm$ to the amplitudes. The condition (3.1) appearing to lowest order in $\hbar$ only requires these coefficients to be of a certain structure, see (3.5). They are, however, completely fixed by the conditions imposed in next-to-leading order. Regarding all higher orders $\hbar^k$, $k = 1, 2, 3, \ldots$, one observes that the equations obtained from the procedure described before (3.1) can be given in a uniform manner. They read

$$\begin{aligned} &\left[H_D\big(\vec{\nabla}_{\vec{x}} S^+, \vec{x}\big) + \frac{\partial S^+}{\partial t} \right] a_k^+(\vec{x}, \vec{y}, t; \vec{\xi}) + \left[c\, \vec{\alpha} \vec{\nabla}_{\vec{x}} + \frac{\partial}{\partial t} \right] a_{k-1}^+(\vec{x}, \vec{y}, t; \vec{\xi}) = 0 \ , \\ &\left[H_D\big(\vec{\nabla}_{\vec{x}} S^-, \vec{x}\big) + \frac{\partial S^-}{\partial t} \right] a_k^-(\vec{x}, \vec{y}, t; \vec{\xi}) + \left[c\, \vec{\alpha} \vec{\nabla}_{\vec{x}} + \frac{\partial}{\partial t} \right] a_{k-1}^-(\vec{x}, \vec{y}, t; \vec{\xi}) = 0 \ . \end{aligned} \tag{3.8}$$

Since these equations, as well as the initial conditions (2.11), are independent of $\vec{y}$, the coefficients $a_k^\pm$ do not depend on $\vec{y}$ either. Beginning with $k = 1$, the hierarchy (3.8) of equations can principally be solved order by order. To this end, for each k we multiply the two equations with $V^\dagger(\vec{\nabla}_{\vec{x}} S^+, \vec{x})$ and $W^\dagger(\vec{\nabla}_{\vec{x}} S^-, \vec{x})$, respectively, from the left. Since $V^\dagger H_D = V^\dagger H^+$ and $W^\dagger H_D = W^\dagger H^-$, the Hamilton-Jacobi equations (3.6) then imply that

$$\begin{aligned} V^\dagger(\vec{\nabla}_{\vec{x}} S^+, \vec{x}) \left[c\, \vec{\alpha} \vec{\nabla}_{\vec{x}} + \frac{\partial}{\partial t} \right] a_{k-1}^+(\vec{x}, \vec{y}, t; \vec{\xi}) = 0 \ , \\ W^\dagger(\vec{\nabla}_{\vec{x}} S^-, \vec{x}) \left[c\, \vec{\alpha} \vec{\nabla}_{\vec{x}} + \frac{\partial}{\partial t} \right] a_{k-1}^-(\vec{x}, \vec{y}, t; \vec{\xi}) = 0 \ . \end{aligned} \tag{3.9}$$

If one started with $a_0^\pm$ as given in (3.5), one now could in principle determine all higher coefficients $a_k^\pm$ from (3.8) and (3.9) recursively. Our ambition is, however, limited to obtain a semiclassical expression for the time evolution kernel to leading order. In the following we therefore restrict our attention to the case $k = 1$ and, moreover, only present the case with index + explicitly.

Expressing a_0^+ as indicated in (3.5), the l.h.s. of the equation (3.9) for $k = 1$ and index + can be viewed as an application of the matrix-valued differential operator

$$V^\dagger(\vec{\nabla}_{\vec{x}} S^+, \vec{x}) \left[c\, \vec{\alpha} \vec{\nabla}_{\vec{x}} + \frac{\partial}{\partial t} \right] V(\vec{\nabla}_{\vec{x}} S^+, \vec{x}) \tag{3.10}$$

to the matrix-valued function $\widetilde{V}(\vec{x}, \vec{\xi}, t)$. A direct calculation shows that (3.10) can be expressed as

$$\vec{\nabla}_{\vec{p}} H^+(\vec{\nabla}_{\vec{x}} S^+, \vec{x}) \vec{\nabla}_{\vec{x}} + \frac{\partial}{\partial t} + \frac{1}{2} \vec{\nabla}_{\vec{x}} \left[\vec{\nabla}_{\vec{p}} H^+(\vec{\nabla}_{\vec{x}} S^+, \vec{x}) \right] + \mathrm{i} M_+(\vec{\nabla}_{\vec{x}} S^+, \vec{x}) \ , \tag{3.11}$$

where we defined the traceless hermitian 2×2 matrix M_+ as

$$M_+(\vec{p}, \vec{x}) := -\frac{ec}{2\varepsilon(\vec{p}, \vec{x})} \left[\vec{B}(\vec{x}) + \frac{c}{\varepsilon(\vec{p}, \vec{x}) + mc^2} \left(\vec{E}(\vec{x}) \times \left(\vec{p} - \frac{e}{c} \vec{A}(\vec{x}) \right) \right) \right] \vec{\sigma} \ . \tag{3.12}$$

We remark that since M_+ is a linear combination of the Pauli matrices, $\mathrm{i}M_+$ is an element of the Lie algebra su(2). In order to emphasize this point, and for later purposes, we introduce the following notation,

$$M_+(\vec{p},\vec{x}) =: \frac{1}{2}\,\vec{R}(\vec{p},\vec{x})\,\vec{\sigma}\ . \tag{3.13}$$

According to the usual convention, the resulting equation for $\widetilde{V}$ is called (first order) transport equation. At this point a comparison with the case of the Schrödinger equation seems to be instructive, see e. g. [40]. There the lowest order amplitude $a_0^{Schr.}$ is a scalar function that is required to be a solution of a transport equation which arises upon acting on $a_0^{Schr.}$ with the equivalent to (3.11), but where $M_+ \equiv 0$. The solution, fixed by the initial condition $a_0^{Schr.} = 1$ at $t = 0$, is well known to be

$$a_0^{Schr.}(\vec{x},\vec{y},t;\vec{\xi}) = \sqrt{\det\left(\frac{\partial^2 S}{\partial x_k \partial \xi_l}(\vec{x},\vec{\xi},t)\right)}\ . \tag{3.14}$$

Returning to the present situation described by (3.11), the following ansatz for the solution of the transport equation therefore seems to be appropriate,

$$\widetilde{V}(\vec{x},\vec{\xi},t) = \sqrt{\det\left(\frac{\partial^2 S^+}{\partial x_k \partial \xi_l}(\vec{x},\vec{\xi},t)\right)}\ U_+(\vec{x},\vec{\xi},t)\ . \tag{3.15}$$

As a consequence, the transport equation for $\widetilde{V}$ implies that the matrix-valued function U_+ has to solve the equation

$$\left[\vec{\nabla}_{\vec{p}} H^+(\vec{\nabla}_{\vec{x}} S^+,\vec{x})\vec{\nabla}_{\vec{x}} + \frac{\partial}{\partial t} + \mathrm{i}M_+(\vec{\nabla}_{\vec{x}} S^+,\vec{x})\right]\ U_+(\vec{x},\vec{\xi},t) = 0\ , \tag{3.16}$$

with initial condition $U_+(\vec{x},\vec{\xi},0) = V^\dagger(\vec{\xi},\vec{x})$.

It is not necessary to solve (3.16) in full generality because the amplitude a_0^+ enters the semiclassical expression for the time evolution only at stationary points $\vec{\xi}_j$ of the phase ϕ^+. We thus first employ the method of stationary phase to the oscillatory integral (2.8), in which we only take the lowest order contributions $a_0^\pm$ to the amplitudes into account. According to (2.14)–(2.17), the stationary points of the phase, i. e., the solutions $\vec{\xi}_j$ of

$$\vec{\nabla}_{\vec{\xi}} \phi^\pm(\vec{x},\vec{y},t;\vec{\xi}_j) = \vec{\nabla}_{\vec{\xi}} S^\pm(\vec{x},\vec{\xi}_j,t) - \vec{y} = 0\ , \tag{3.17}$$

determine solutions $(\vec{P}(t';\vec{\xi}_j,\vec{y}),\vec{X}(t';\vec{\xi}_j,\vec{y}))$, $0 \le t' \le t$, of the classical equations of motion from $(\vec{\xi}_j,\vec{y})$ to $(\vec{p},\vec{x})$ in time t. Their projections $\vec{X}(t';\vec{\xi}_j,\vec{y})$ to configuration space will also be denoted as $\gamma_{xy}^\pm$. At a stationary point the phase is given by Hamilton's principal function for the trajectory $\gamma_{xy}^\pm$ corresponding to $\vec{\xi}_j$,

$$\phi^\pm(\vec{x},\vec{y},t;\vec{\xi}_j) = S^\pm(\vec{x},\vec{\xi}_j,t) - \vec{y}\vec{\xi}_j = \int_0^t L^\pm\left(\vec{X}(t'),\dot{\vec{X}}(t')\right)\mathrm{d}t' =: R^\pm_{\gamma_{xy}^\pm}(\vec{x},\vec{y},t)\ , \tag{3.18}$$

where $L^{\pm}$ is the Lagrangian associated with $H^{\pm}$.

The method of stationary phase requires the amplitudes $a_0^{\pm}$, and hence $U_{\pm}$, evaluated at the stationary points $\vec{\xi}_j$. In this situation $\vec{x}$ has to be considered as the end point of the corresponding trajectory γ_{xy}^+, i. e., $\vec{x} = \vec{X}(t)$. In (3.16) the first two terms can therefore be understood as a total time derivative along $\vec{X}(t)$,

$$\vec{\nabla}_{\vec{p}} H^+(\vec{P}(t), \vec{X}(t)) \vec{\nabla}_{\vec{x}} + \frac{\partial}{\partial t} = \dot{\vec{X}}(t) \vec{\nabla}_{\vec{x}} + \frac{\partial}{\partial t} =: \frac{\mathrm{d}}{\mathrm{d}t} \,. \tag{3.19}$$

In order to solve (3.16) at a stationary point $\vec{\xi}_j$ we now introduce the ansatz

$$U_+(\vec{X}(t), \vec{\xi}_j, t) = d_+(\vec{P}(t), \vec{X}(t))\, V^\dagger(\vec{\xi}_j, \vec{y}) \;, \tag{3.20}$$

which immediately implies the initial condition

$$d_+(\vec{P}(0), \vec{X}(0)) = \mathbb{1}_2 \tag{3.21}$$

for the 2×2 matrix d_+. Restricting (3.16) to the trajectory $\vec{X}(t)$ and using the abbreviation (3.19) then shows that this matrix is required to solve

$$\left[\frac{\mathrm{d}}{\mathrm{d}t} + \mathrm{i} M_+(\vec{P}(t), \vec{X}(t)) \right] d_+(\vec{P}(t), \vec{X}(t)) = 0 \tag{3.22}$$

along the trajectory. In the next section we will demonstrate that d_+ can be interpreted as a semiclassical propagator for the spin degrees of freedom. Occasionally, we will thus refer to (3.22) as the spin transport equation. A formal solution of this equation can be given in terms of a time-ordered exponential,

$$d_+(t) = \mathrm{T}\, \exp \left\{ -\mathrm{i} \int_0^t M_+(t')\, \mathrm{d}t' \right\} \;. \tag{3.23}$$

Since according to (3.12) $\mathrm{i}M_+$ takes values in the Lie algebra su(2), the solution d_+ is an element of the group SU(2). Together with its connection to a classical spin, a further geometric interpretation of d_+ will be provided in the next section.

Combining (3.5), (3.15), and (3.20) finally yields the lowest-order amplitude at a stationary point as

$$\begin{aligned} a_0^+(\vec{x}, \vec{y}, t; \vec{\xi}_j) = & \sqrt{\det \left(\frac{\partial^2 S^+}{\partial x_k \partial \xi_l}(\vec{x}, \vec{\xi}_j, t) \right)} \\ & V\big(\vec{\nabla}_{\vec{x}} S^+(\vec{x}, \vec{\xi}_j, t), \vec{x}\big)\, d_+\big(\vec{\nabla}_{\vec{x}} S^+(\vec{x}, \vec{\xi}_j, t), \vec{x}\big)\, V^\dagger(\vec{\xi}_j, \vec{y}) \;. \end{aligned} \tag{3.24}$$

This expression has an obvious analogue for the index $-$, for which the 2×2 matrix M_- is given by

$$M_-(\vec{p}, \vec{x}) := \frac{ec}{2\varepsilon(\vec{p}, \vec{x})} \left[\vec{B}(\vec{x}) - \frac{c}{\varepsilon(\vec{p}, \vec{x}) + mc^2} \left(\vec{E}(\vec{x}) \times \left(\vec{p} - \frac{e}{c} \vec{A}(\vec{x}) \right) \right) \right] \vec{\sigma} \;. \tag{3.25}$$

Comparing (3.24) with (3.14) reveals that, apart from the occurrence of two classical Hamiltonians, the only difference to the case of the semiclassical propagator for the Schrödinger equation is given by the appearence of the last three factors on the r.h.s. of (3.24), which we also abbreviate as $V_t\, d_+ V_0^\dagger$. With the further short-hand

$$D_{\gamma_{xy}^\pm} := \left|\det\left(-\frac{\partial^2 R^\pm_{\gamma_{xy}^\pm}}{\partial x_k \partial y_l}(\vec{x},\vec{y},t)\right)\right|^{1/2} \tag{3.26}$$

the result of the method of stationary phase applied to (2.8) finally reads (for $t \neq 0$)

$$\begin{aligned} K(\vec{x},\vec{y},t) = \frac{1}{(2\pi \mathrm{i}\hbar)^{3/2}} \Bigg\{ &\sum_{\gamma_{xy}^+} V_t\, d_+ V_0^\dagger\, D_{\gamma_{xy}^+}\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar} R^+_{\gamma_{xy}^+} - \mathrm{i}\frac{\pi}{2}\nu_{\gamma_{xy}^+}} \left[1 + O(\hbar)\right] \\ &+ \sum_{\gamma_{xy}^-} W_t\, d_- W_0^\dagger\, D_{\gamma_{xy}^-}\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar} R^-_{\gamma_{xy}^-} - \mathrm{i}\frac{\pi}{2}\nu_{\gamma_{xy}^-}} \left[1 + O(\hbar)\right] \Bigg\} \;, \end{aligned} \tag{3.27}$$

where, as in the case of the Schrödinger equation, $\nu_{\gamma_{xy}^\pm}$ denotes the Morse index of the trajectory $\gamma_{xy}^\pm$. Notice that the two sums extend over the classical trajectories of relativistic point particles. The spin degrees of freedom, which manifest themselves in the Dirac equation through the matrix character of the Hamiltonian, enter in leading semiclassical order only through the factors $V_t\, d_+ V_0^\dagger$ and $W_t\, d_- W_0^\dagger$, respectively. Since these contain no $\hbar$, a classical interpretation of them seems to be in order. In the next section we will indeed obtain from (3.22) an evolution equation for a classical spin which is transported through the external fields along the particle trajectories $\gamma_{xy}^\pm$.

As our final step in this section, we now modify (3.27) to yield a semiclassical representation for the truncated time evolution kernel K_χ. According to (2.22), to this end one must apply the 4×4 matrix $\chi(H_D(\vec{\nabla}_{\vec{x}} S^\pm, \vec{x}))$ to the ampliude $a_0^\pm(\vec{x},\vec{y},t;\xi)$. Since the spectral representation $H_D = H^+ P_+ + H^- P_-$ of the symbol matrix implies

$$\chi(H_D) = \chi(H^+)\, P_+ + \chi(H_-)\, P_- = \chi(H^+)\, V\, V^\dagger + \chi(H^-)\, W\, W^\dagger \;, \tag{3.28}$$

representing the amplitudes as in (3.5) immediately shows that

$$\chi(H_D)\, a_0^\pm = \chi(H^\pm)\, a_0^\pm \;. \tag{3.29}$$

Since therefore the matrix-valued amplitudes are only multiplied by a scalar factor, which is moreover constant along any classical trajectory $\gamma_{xy}^\pm$, the only modification of (3.27) consists of an inclusion of the factors $\chi(E_{\gamma_{xy}^\pm})$ under the sums over the trajectories, where $E_{\gamma_{xy}^\pm} = H^\pm(\vec{P}(t), \vec{X}(t))$ denotes the (constant) energy of $\gamma_{xy}^\pm$.

4 Geometry of semiclassical spin transport

The semiclassical representation for the time evolution kernel that was derived in the previous section is principally determined by the classical dynamics of relativistic point particles.

This is true to the extent that it essentially suffices to solve the equations of motion generated by the scalar Hamiltonians $H^\pm$. Indeed, the semiclassically dominating $\hbar$-dependent phases occurring in (3.27) are completely fixed by Hamilton's principal functions $R^\pm$ of the translational motion. The latter decouples from the spin dynamics that, moreover, only contributes to the $\hbar$-independent amplitudes in (3.27).

In this section we will investigate the dynamics of the spin degrees of freedom more closely. In particluar, we will interpret the SU(2) matrix d_+ as a semiclassical time evolution operator for spin and, furthermore, relate it to a classical spin evolving according to a classical equation of motion. In order to prepare for this, we first have to clarify the geometrical setting of spin transport along classical particle trajectories further. To this end we consider the H^+-eigenbundle E^+ over phase space. It is defined as the disjoint collection of the eigenspaces

$$E^+_{(\vec{p},\vec{x})} := P_+(\vec{p},\vec{x})\,\mathbb{C}^4 \tag{4.1}$$

of the symbol matrix $H_D(\vec{p},\vec{x})$ corresponding to the eigenvalue $H^+(\vec{p},\vec{x})$ for each point $(\vec{p},\vec{x})$ in phase space. Since H_D is hermitian, the decomposition of $\mathbb{C}^4$ into the H^+- and H^--eigenspaces is orthogonal with respect to the canonical scalar product. This can hence be projected to the fibres $E^+_{(\vec{p},\vec{x})}$, so that E^+ is a $\mathbb{C}^2$ vector bundle with structure group U(2). In terms of the orthonormal basis $\{e_1(\vec{p},\vec{x}), e_2(\vec{p},\vec{x})\}$ used to define the matrix $V(\vec{p},\vec{x})$ in (3.2), a section in the eigenbundle can be represented as

$$v(\vec{p},\vec{x}) = \sum_{k=1}^{2} v_k(\vec{p},\vec{x})\, e_k(\vec{p},\vec{x}) = V(\vec{p},\vec{x}) \begin{pmatrix} v_1(\vec{p},\vec{x}) \\ v_2(\vec{p},\vec{x}) \end{pmatrix} \ . \tag{4.2}$$

To lowest semiclassical order the spin dynamics is governed by the transport equation defined with the differential operator (3.10). This requires sections in the eigenbundle E^+ that are lifts of trajectories in phase space. We therefore now consider the following differentiation on sections v, which we evaluate at $(\vec{p},\vec{x}) = (\vec{\nabla}_{\vec{x}} S^+(\vec{x},\vec{\xi},t),\vec{x})$. Then

$$\begin{aligned} \tilde{v}(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) &:= P_+(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) \left[c\vec{\alpha}\vec{\nabla}_{\vec{x}} + \frac{\partial}{\partial t}\right] v(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) \\ &= V(\vec{\nabla}_{\vec{x}}S^+,\vec{x})\, V^\dagger(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) \left[c\vec{\alpha}\vec{\nabla}_{\vec{x}} + \frac{\partial}{\partial t}\right] V(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) \begin{pmatrix} v_1(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) \\ v_2(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) \end{pmatrix} \end{aligned} \tag{4.3}$$

is again a section in E^+ in the above sense. According to (3.10) and (3.11) an expansion of $\tilde{v}$ in the gliding basis $\{e_1, e_2\}$ yields the coefficients

$$\begin{aligned} \begin{pmatrix} \tilde{v}_1(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) \\ \tilde{v}_2(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) \end{pmatrix} = \Bigg(&\vec{\nabla}_{\vec{p}}H^+(\vec{\nabla}_{\vec{x}}S^+,\vec{x})\vec{\nabla}_{\vec{x}} + \frac{\partial}{\partial t} + \frac{1}{2}\vec{\nabla}_{\vec{x}}\left[\vec{\nabla}_{\vec{p}}H^+(\vec{\nabla}_{\vec{x}}S^+,\vec{x})\right] \\ &+ \mathrm{i}M_+(\vec{\nabla}_{\vec{x}}S^+,\vec{x})\Bigg) \begin{pmatrix} v_1(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) \\ v_2(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) \end{pmatrix} \ . \end{aligned} \tag{4.4}$$

Furthermore, a separation analogous to (3.15),

$$v(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) = \sqrt{\det\left(\frac{\partial^2 S^+}{\partial x_k \partial \xi_l}(\vec{x},\vec{\xi},t)\right)}\, u(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) \ , \tag{4.5}$$

leads via (3.16) to the definition of a covariant differentiation $\mathcal{D}^+$ on the section u,

$$\begin{aligned}&\mathcal{D}^+ u(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) := \\ &\quad V(\vec{\nabla}_{\vec{x}}S^+,\vec{x})\left(\vec{\nabla}_{\vec{p}}H^+(\vec{\nabla}_{\vec{x}}S^+,\vec{x})\vec{\nabla}_{\vec{x}} + \frac{\partial}{\partial t} + \mathrm{i}M_+(\vec{\nabla}_{\vec{x}}S^+,\vec{x})\right)\begin{pmatrix} u_1(\vec{\nabla}_{\vec{x}}S^+,\vec{x}) \\ u_2(\vec{\nabla}_{\vec{x}}S^+,\vec{x})\end{pmatrix} \ .\end{aligned} \tag{4.6}$$

If one now restricts the variable $\vec{\xi}$ to the stationary points $\vec{\xi}_j$ arising in (3.17), the first two terms in (4.6) again yield a differentiation along the trajectory γ^+_{xy} associated with $\vec{\xi}_j$, compare (3.22). One then also recognizes $\mathrm{i}M_+$ as the su(2)-valued connection coefficient arising for the connection associated with $\mathcal{D}^+$. A section u given along a solution of the classical equations of motion is therefore parallel, if it is a solution of

$$\mathcal{D}^+ u(\vec{P}(t),\vec{X}(t)) = 0 \quad \text{with} \quad u_k(\vec{P}(0),\vec{X}(0)) = u_{k,0} \ . \tag{4.7}$$

According to (3.22) such a solution can also be represented as

$$\begin{pmatrix} u_1(\vec{P}(t),\vec{X}(t)) \\ u_2(\vec{P}(t),\vec{X}(t))\end{pmatrix} = d_+(\vec{P}(t),\vec{X}(t)) \begin{pmatrix} u_{1,0} \\ u_{2,0}\end{pmatrix} \ . \tag{4.8}$$

Thus, geometrically $d_+ \in \mathrm{SU}(2)$ describes the parallel transport in E^+ defined by the connection arising from $\mathcal{D}^+$. Along periodic orbits in phase space, d_+ therefore yields the holonomy of this connection. This geometric interpretation ensures that the combination $V_t\, d_+\, V_0^\dagger$, which appears in the semiclassical expression (3.27) for the time evolution kernel, is invariant under unitary base changes in E^+. In physical terms, d_+ can be interpreted as the semiclassical time evolution operator for two-spinors in the representation defined via the gliding basis $\{e_1, e_2\}$. The unitarity of d_+ then implies that the norm $|u_{1,0}|^2 + |u_{2,0}|^2$ of the initial two-spinor $(u_{1,0}, u_{2,0})^T \in \mathbb{C}^2$ is preserved under this evolution. In the following we will therefore always consider normalised sections u in E^+.

We would now like to compare the above construction with the connections that appear in the analysis of Littlejohn and Flynn [7], and Emmrich and Weinstein [8]. Since the eigenbundle E^+ is a (non-trivial) subbundle of the trivial $\mathbb{C}^4$ bundle over phase space, a natural connection in E^+ arises by projecting the trivial covariant differentiation of the $\mathbb{C}^4$ bundle to E^+. Along a trajectory $(\vec{P}(t),\vec{X}(t))$ this construction reads

$$P_+(\vec{P}(t),\vec{X}(t))\left[\frac{\mathrm{d}}{\mathrm{d}t}u(\vec{P}(t),\vec{X}(t))\right] =: \mathcal{D}^B u(\vec{P}(t),\vec{X}(t)) \ , \tag{4.9}$$

when applied to a section u in E^+. In analogy to (4.6) one then obtains a covariant differentiation in terms of the coefficients u_k with respect to the gliding basis $\{e_1, e_2\}$. The connection coefficient $\mathrm{i}M_B$ that replaces $\mathrm{i}M_+$ can be calculated as

$$
\begin{aligned}
M_B(\vec{p},\vec{x}) =& \frac{ec^2}{2\,\varepsilon(\vec{p},\vec{x})[\varepsilon(\vec{p},\vec{x})+mc^2]} \left[(\vec{p}-\tfrac{e}{c}\vec{A}(\vec{x}))\times\vec{E}(\vec{x})\right]\vec{\sigma} \\
&+ \frac{ec^3}{2\,\varepsilon^2(\vec{p},\vec{x})[\varepsilon(\vec{p},\vec{x})+mc^2]} \left[(\vec{p}-\tfrac{e}{c}\vec{A}(\vec{x}))\times\big((\vec{p}-\tfrac{e}{c}\vec{A}(\vec{x}))\times\vec{B}(\vec{x})\big)\right]\vec{\sigma}\ .
\end{aligned}
\tag{4.10}
$$

That way one defines a connection on E^+ that bears some similarities to the adiabatic connection in quantum mechanics. The latter has been identified by Simon [30] to produce the Berry phase [29], see also [8]. On this ground, Littlejohn and Flynn [6, 7] introduced the notion of a Berry term for the analogue to our M_B in the case of principal symbol matrices with no globally degenerate eigenvalues. In the present context, the twofold degenerate eigenvalue H^+ forces M_B to take values in su(2), which hence leads to a connection with SU(2) holonomy. We emphasize, however, that no adiabatic approximation is made after one has arrived at the transport equations (3.8) and (3.16), respectively. Nevertheless, following [6, 7] in spirit, we refer to M_B as the SU(2)-Berry term, although regarding adiabatic approximations this notation is sligthly misleading.

The difference between the two covariant differentiations $\mathcal{D}^+$ and $\mathcal{D}^B$ can be expressed in terms of a connection coefficient $M_C = M_+ - M_B$. This expression, which Littlejohn and Flynn [7] refer to as the no-name term, has been identified by Emmrich and Weinstein [8] to be related to the curvature associated with $\mathcal{D}^B$. They moreover showed that

$$
M_C(\vec{p},\vec{x}) = -\frac{\mathrm{i}}{2} V^\dagger(\vec{p},\vec{x})\,\{P_+, H_D - H^+\mathbb{1}_4\}(\vec{p},\vec{x})\ V(\vec{p},\vec{x})\ , \tag{4.11}
$$

where the Poisson bracket for two matrix-valued functions A, B on phase space is defined as

$$
\{A,B\}(\vec{p},\vec{x}) := \vec{\nabla}_{\vec{p}}A(\vec{p},\vec{x})\,\vec{\nabla}_{\vec{x}}B(\vec{p},\vec{x}) - \vec{\nabla}_{\vec{p}}B(\vec{p},\vec{x})\,\vec{\nabla}_{\vec{x}}A(\vec{p},\vec{x})\ . \tag{4.12}
$$

Notice that the ordering of the matrices is important. Upon explicitly calculating the r.h.s. of (4.11) one can verify that $M_+ = M_B + M_C$.

We now define a time-dependent spin operator $\vec{\Sigma}(t)$, whose components act on $\mathbb{C}^2$, as

$$
\vec{\Sigma}(t) := d_+^\dagger(\vec{P}(t),\vec{X}(t))\,\vec{\sigma}\,d_+(\vec{P}(t),\vec{X}(t))\ , \tag{4.13}
$$

so that $\vec{\Sigma}(0) = \vec{\sigma}$. According to (3.22), the dynamics of the spin operator $\vec{\Sigma}(t)$ is governed by

$$
\frac{\mathrm{d}}{\mathrm{d}t}\vec{\Sigma}(t) = \mathrm{i}\,d_+^\dagger(t)\,[M_+(t)\,\vec{\sigma} - \vec{\sigma}\,M_+(t)]\,d_+(t)\ . \tag{4.14}
$$

Introducing $\vec{R}(\vec{p},\vec{x})$ as in (3.13), the evolution equation for $\vec{\Sigma}$ can be brought into the convenient form

$$
\frac{\mathrm{d}}{\mathrm{d}t}\vec{\Sigma}(t) = \vec{R}(t)\times\vec{\Sigma}(t)\ , \tag{4.15}
$$

which describes the precession of the vector $\vec{\Sigma}$ about the instantaneous axis defined by $\vec{R}$. In order to obtain an object that can be considered as a classical spin, one introduces the expectation value of $\vec{\Sigma}$ in a two-spinor state prescribed by $(u_{1,0}, u_{2,0})^T \in \mathbb{C}^2$,

$$\vec{s}(t) := (\overline{u}_{1,0}, \overline{u}_{2,0})\, \vec{\Sigma}(t) \begin{pmatrix} u_{1,0} \\ u_{2,0} \end{pmatrix} = (\overline{u}_1(t), \overline{u}_2(t))\, \vec{\sigma} \begin{pmatrix} u_1(t) \\ u_2(t) \end{pmatrix} = \begin{pmatrix} 2\ \mathrm{Re}(\overline{u}_1(t)\, u_2(t)) \\ 2\ \mathrm{Im}(\overline{u}_1(t)\, u_2(t)) \\ |u_1(t)|^2 - |u_2(t)|^2 \end{pmatrix} , \quad (4.16)$$

which obviously also solves (4.15), i. e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{s} = \vec{s} \times \left(\frac{ec}{\varepsilon}\vec{B} - \frac{ec^2}{\varepsilon(\varepsilon + mc^2)} \left(\vec{p} - \frac{e}{c}\vec{A} \right) \times \vec{E} \right) , \quad (4.17)$$

where all quantities have to be taken along a given trajectory γ^+_{xy}. This classical equation is well known to describe the precession of a spinning particle in external electromagnetic fields $\vec{E}$ and $\vec{B}$, as has already been demonstrated by Thomas [27]. In [28] it is rederived in a manifestly covariant formulation, and therefore also goes under the notion of BMT equation. In the present context, (4.17) can be viewed as a manifestation of the Ehrenfest theorem for spin because here $\vec{s}$ stands for any expectation value of the spin operator $\vec{\Sigma}$. Notice that since we deliberately omitted a factor of $\hbar/2$ in the definition (4.13) of the spin operator, the classical spin vector $\vec{s}$ is of (constant) unit length.

So far we have provided geometrical and physical interpretations of d_+. Yet, for the purpose of the semiclassical representation (3.27) of the time evolution kernel one needs to calculate the SU(2) matrix

$$d_+(\vec{P}(t), \vec{X}(t)) =: \begin{pmatrix} \alpha(t) & -\overline{\beta}(t) \\ \beta(t) & \overline{\alpha}(t) \end{pmatrix} , \qquad |\alpha(t)|^2 + |\beta(t)|^2 = 1 , \quad (4.18)$$

for each classical trajectory γ^+_{xy}. This can be achieved along the lines presented above, if one chooses the initial condition $u(\vec{\xi}_j, \vec{y}) = e_1(\vec{\xi}_j, \vec{y})$ for a section u solving $\mathcal{D}^+ u = 0$. In the two-spinor representation for u this initial condition reads $(u_{1,0}, u_{2,0}) = (1, 0)$, and thus (4.8) implies that

$$\begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix} = \begin{pmatrix} u_1(\vec{P}(t), \vec{X}(t)) \\ u_2(\vec{P}(t), \vec{X}(t)) \end{pmatrix} . \quad (4.19)$$

The spin expectation value $\vec{s}(t)$ corresponding to this choice then follows from (4.16) as

$$\vec{s}(t) = (\overline{\alpha}(t), \overline{\beta}(t))\, \vec{\sigma} \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix} = \begin{pmatrix} 2\ \mathrm{Re}(\overline{\alpha}(t)\, \beta(t)) \\ 2\ \mathrm{Im}(\overline{\alpha}(t)\, \beta(t)) \\ |\alpha(t)|^2 - |\beta(t)|^2 \end{pmatrix} , \quad \text{with} \quad \vec{s}(0) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} . \quad (4.20)$$

Mathematically, this physically motivated construction can be viewed as a map from $d_+ \in \mathrm{SU}(2)$ to $\vec{s} \in \mathrm{S}^2 \subset \mathbb{R}^3$. Indeed, it is known as the Hopf map $\pi_H : \mathrm{SU}(2) \to \mathrm{S}^2$, which yields a U(1) principal fibre bundle over S^2.

In order to calculate $d_+(t)$ for a given trajectory γ_{xy}^+ one first has to integrate the evolution equation (4.17) for the precession of a classical spin along γ_{xy}^+ with initial condition $\vec{s}(0) = (0,0,1)^T$. According to the relation $\vec{s}(t) = \pi_H(d_+(t))$ one thus has determined two of the three real degrees of freedom of $d_+(t)$ by classical means. The third degree of freedom can only be reconstructed, if one is able to lift the curve $\vec{s}(t)$ in S^2 to $\mathrm{SU}(2)$. To this end one requires a connection on the $\mathrm{U}(1)$ bundle over S^2 that is provided by the Hopf map. The two degrees of freedom of the classical spin $\vec{s}$ can be related to convenient coordinates on S^2 once one notices that the normalisation forces $|\alpha|$ to range in the interval $[0,1]$. Therefore, a variable $\theta \in [0,\pi]$ can be introduced such that

$$|\alpha| = \cos\tfrac{\theta}{2} \qquad \text{and} \qquad |\beta| = \sin\tfrac{\theta}{2} \ . \tag{4.21}$$

Together with the phases of $\alpha = |\alpha|\,\mathrm{e}^{\mathrm{i}\eta}$ and $\beta = |\beta|\,\mathrm{e}^{\mathrm{i}\lambda}$ one thus has three degrees of freedom at hand to describe d_+. A representation of the classical spin $\vec{s}$ in terms of the variables (θ,η,λ) then follows from (4.20),

$$\vec{s} = \begin{pmatrix} \sin\theta\,\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} \ , \quad \text{with} \quad \phi := \lambda - \eta \ , \tag{4.22}$$

so that (θ,ϕ) can be identified as the usual spherical coordinates on S^2. In principle, one could now choose $\lambda+\eta$ as the additional spin degree of freedom discussed above. However, in order to identify the connection on the Hopf fibration it turns out that a choice of either η or λ separately is more approppriate. Since the north pole of S^2 corresponds to $(\alpha_N,\beta_N) = (1,0)$ and the south pole to $(\alpha_S,\beta_S) = (0,1)$, the phase η is ill-defined at the south pole, whereas λ is ill-defined at the north pole. Following the procedure well known from the analysis of magnetic monopoles by Wu and Yang [43], we now choose η as a fibre coordinate for base points on the northern hemisphere $U_N \subset \mathrm{S}^2$ and, correspondingly, λ for base points on the southern hemisphere $U_S \subset \mathrm{S}^2$. Since the connection we want to identify is fixed by the requirement that the lifted curve on $\mathrm{SU}(2)$ be the solution $d_+(t)$ of (3.22), an explicit expression for the connection coefficients can be derived from the equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\alpha(t)\\ \beta(t)\end{pmatrix} = -\mathrm{i}M_+(t)\begin{pmatrix}\alpha(t)\\ \beta(t)\end{pmatrix} \tag{4.23}$$

that follows from the identification (4.19). Multiplying this with $(\overline{\alpha}(t),\overline{\beta}(t))$ from the left now yields

$$|\alpha(t)|^2\frac{\mathrm{d}}{\mathrm{d}t}\eta(t) + \left(1-|\alpha(t)|^2\right)\frac{\mathrm{d}}{\mathrm{d}t}\lambda(t) = -\frac{1}{2}\,\vec{R}(t)\vec{s}(t) \ . \tag{4.24}$$

Exploiting (4.21) and (4.22) then results in equations for η on U_N and λ on U_S, respectively,

$$\frac{\mathrm{d}}{\mathrm{d}t}\eta(t) = -\frac{1}{2}\,\vec{R}(t)\vec{s}(t) - \frac{1}{2}\left(1-\cos\theta(t)\right)\frac{\mathrm{d}}{\mathrm{d}t}\phi(t) \ , \tag{4.25}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\lambda(t) = -\frac{1}{2}\,\vec{R}(t)\vec{s}(t) + \frac{1}{2}\left(1+\cos\theta(t)\right)\frac{\mathrm{d}}{\mathrm{d}t}\phi(t) \ . \tag{4.26}$$

According to the initial condition in (4.20) the motion of the classical spin $\vec{s}$ starts at the north pole so that for sufficiently small times $\vec{s}(t) \in U_N$. Thus the phase η should be used, whose initial condition $\eta(0) = 0$ follows from (3.21). This allows an immediate integration of (4.25),

$$\eta(t) = -\frac{1}{2}\int_0^t \vec{R}(t')\vec{s}(t')\,\mathrm{d}t' - \frac{1}{2}\int_0^t \big(1-\cos\theta(t')\big)\,\frac{\mathrm{d}\phi}{\mathrm{d}t'}(t')\,\mathrm{d}t' \ . \tag{4.27}$$

The first term on the r.h.s. of (4.27) is a dynamical phase associated with the classical energy of a magnetic moment in given electromagnetic fields, whereas the second term[1] is a geometric phase. The latter can be further characterised once one takes into account that η is ill-defined at the south pole so that the phase λ should be used instead of η as soon as $\vec{s}$ enters U_S, say, at a time t_0. One then has to integrate (4.26) with initial condition $\lambda(t_0) = \phi(t_0) + \eta(t_0)$. To this end the one-form $-\frac{1}{2}(1-\cos\theta)\mathrm{d}\phi$, which constitutes the geometric part of (4.27), has to be replaced by $\frac{1}{2}(1+\cos\theta)\mathrm{d}\phi$, see (4.26). Since these two expressions are the gauge potentials of a magnetic monopole, see [43], we can now formally identify the geometric part of (4.27) to be caused by a magnetic monopole of strength $-1/2$ situated at the origin of the sphere. We again emphasize that in the above consideration no adiabaticity assumption was made. Therefore, although the result for the geometric phase is strikingly similar to the Berry phase of a precessing quantum mechanical spin [29], the geometric part of η is rather of the more general type discussed by Aharonov and Anandan [32].

Having integrated the equations for the classical spin and for the additional phase, we are now able to present the SU(2) matrix d_+ in the form

$$d_+(\vec{P}(t),\vec{X}(t)) = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right)\mathrm{e}^{\mathrm{i}\eta} & -\sin\left(\frac{\theta}{2}\right)\mathrm{e}^{-\mathrm{i}(\eta+\phi)} \\ \sin\left(\frac{\theta}{2}\right)\mathrm{e}^{\mathrm{i}(\eta+\phi)} & \cos\left(\frac{\theta}{2}\right)\mathrm{e}^{-\mathrm{i}\eta} \end{pmatrix}, \tag{4.28}$$

where (θ,ϕ) are spherical coordinates for $\vec{s}(t)$, and η is given by (4.27), if $\vec{s}(t) \in U_N$, and by $\eta(t) = \lambda(t) - \phi(t)$, if $\vec{s}(t) \in U_S$. With this explicit formula for d_+ all terms entering the semiclassical propagator (3.27) to leading order in $\hbar$ are completely defined in terms of classical quantities.

5 Semiclassical trace formula

After having obtained the fairly explicit expression (3.27) for the time evolution kernel together with an interpretation in terms of classical quantities, our ultimate goal now is to set up a semiclassical trace formula for the Dirac equation. In the case of the Schrödinger equation, Gutzwiller's original approach was to express the quantum mechanical density of states in terms of a sum over classical periodic orbits (or, more generally, over connected manifolds of periodic points of the classical flow). To this end he Fourier-transformed the

[1] We remark that in contrast to equation (21) of our recent Letter [44] the sign of this term should be as in (4.27).

semiclassical expression for the retarded time evolution kernel, which he derived from its path integral representation, in order to obtain a semiclassical approximation for the Green function. Subsequently he performed the trace integral with the method of stationary phase. The result then immediately yielded the semiclassical spectral density, see [10] for details. Since that way one has to deal with several singular objects, we here prefer to derive a regularised trace formula that only takes finite quantities into account. The key relation for this procedure is equation (2.27), in which we below use a semiclassical representation for the truncated time evolution kernel $K_\chi(\vec{x},\vec{y},t)$. We prefer this procedure, since first of all the energy localisation introduced through the truncation χ ensures that only the point spectrum of $\hat{H}_D$ contributes. Secondly, the test function $\tilde{\varrho}$ cuts off all periods of classical periodic orbits that exceed some maximal value T_{max}, since we request $\tilde{\varrho}$ to be compactly supported. This cut-off prohibits any possible clash of the two non-commuting asymptotics $\hbar \to 0$ and $t \to \infty$. Later $\tilde{\varrho}$ can be chosen to have an arbitrarily large, though compact, support. Possibly, this support condition can be weakened by demanding a sufficiently strong decrease of $\tilde{\varrho}(t)$ as $|t| \to \infty$, see [45, 16].

The semiclassical analysis presented at the end of section 2 already revealed that, as $\hbar \to 0$, all contributions to (2.27) which exceed $O(\hbar^\infty)$ have to derive from classical periodic orbits $\gamma_p^\pm$. These are associated with the stationary points $(\vec{\xi}_{\gamma_p^\pm},\vec{x}_{\gamma_p^\pm},T_{\gamma_p^\pm})$ of the phase $\phi^\pm + Et$ appearing in the integral (2.28). We also pointed out that the manifolds $M_0^\pm$ of stationary points $(\vec{\xi}_0,\vec{x}_0,0)$ are related to the hypersurfaces $\Omega_E^\pm$ of constant energy, which are composed of periodic points with trivial periods $T_0 = 0$. We now assume the cleanness condition explained in section 2 and recall that in particular this implies that all further stationary points are such that the periods $T_{\gamma_p^\pm}$ do not accumulate at $t = 0$. It is then possible to choose a smooth function $h \in C_0^\infty(\mathbb{R})$ whose (connected) support contains the period $T_0 = 0$, but no further period $T_{\gamma_p^\pm} > 0$. We furthermore require h to fulfill $h(t) = 1$ on some neighbourhood of $T_0 = 0$. Upon introducing the partition of unity $1 = h(t) + [1 - h(t)]$ under the integral (2.27), the stationary points $(\vec{\xi}_0,\vec{x}_0,0)$ are separated from the further stationary points $(\vec{\xi}_{\gamma_p^\pm},\vec{x}_{\gamma_p^\pm},T_{\gamma_p^\pm})$ associated with the non-trivial periodic orbits $\gamma_p^\pm$. These two classes of stationary points will contribute to (2.27) in essentially different ways so that we will deal with them separately. Let our first concern hence be the calculation of the leading order contribution of the stationary points $(\vec{\xi}_0,\vec{x}_0,0)$. We therefore consider the integral

$$\begin{aligned}\frac{1}{2\pi(2\pi\hbar)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{-\infty}^{+\infty} h(t)\,\tilde{\varrho}(t)\ \mathrm{tr}\Big[\chi\left(H_D(\vec{\nabla}_{\vec{x}}\phi^+,\vec{x})\right)\,a_0^+\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\phi^+ + Et)} \\ +\chi\left(H_D(\vec{\nabla}_{\vec{x}}\phi^-,\vec{x})\right)\,a_0^-\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\phi^- + Et)}\Big]\ \mathrm{d}t\,\mathrm{d}^3\xi\,\mathrm{d}^3x\ .\end{aligned} \tag{5.1}$$

Since the cut-off function h ensures that no stationary points with $t \neq 0$ contribute, we expand the phases about $t = 0$. Using the Hamilton-Jacobi equation for $S^\pm(\vec{x},\vec{\xi},t)$, one finds

$$
\begin{aligned}
\phi^{\pm}(\vec{x},\vec{x},t;\vec{\xi}) + Et &= S^{\pm}(\vec{x},\vec{\xi},t) + Et - \vec{x}\vec{\xi} \\
&= t\left[E + \frac{\partial S^{\pm}}{\partial t}(\vec{x},\vec{\xi},0)\right] + \frac{t^2}{2}\frac{\partial^2 S^{\pm}}{\partial t^2}(\vec{x},\vec{\xi},0) + O(t^3) \\
&= t\left[E - H^{\pm}(\vec{\xi},\vec{x})\right] + \frac{t^2}{2}\vec{\nabla}_{\vec{p}}H^{\pm}(\vec{\xi},\vec{x})\,\vec{\nabla}_{\vec{x}}H^{\pm}(\vec{\xi},\vec{x}) + O(t^3)\ .
\end{aligned}
\tag{5.2}
$$

At this stage we introduce in (5.1) polar coordinates for the variable $\vec{\xi}$, i. e., $\vec{\xi} = \lambda\omega$ with $\lambda := |\vec{\xi}|$ and solid angle $\omega \in \mathrm{S}^2 \subset \mathbb{R}^3$. This implies $d^3\xi = \lambda^2\, d\lambda\, d\omega$. We then employ the method of stationary phase to the integration over the variables $(t,\lambda) \in \mathbb{R}\times\mathbb{R}^+$. Stationary points are therefore determined by a vanishing of the derivatives of (5.2) with respect to t and λ, respectively. Evaluated at $t = 0$, the expression (5.2) shows that this yields the condition $H^{\pm}(\lambda_0^{\pm}\omega, x) = E$ to be fulfilled by the stationary points $(t_0^{\pm} = 0, \lambda_0^{\pm})$. Therefore, our first conclusion is that the integral over the remaining variables $(\vec{x},\omega) \in \mathbb{R}^3 \times \mathrm{S}^2$ is in fact restricted to the hypersurfaces Ω_E^+ and Ω_E^-, respectively. Carrying out the method of stationary phase further finally yields an asymptotic expansion of the integral (5.1) as $\hbar \to 0$ whose leading term can be determined explicitly in a straight forward manner,

$$
\chi(E)\,\frac{\tilde{\varrho}(0)}{2\pi}\,\frac{2\mathrm{vol}\,(\Omega_E^+) + 2\mathrm{vol}\,(\Omega_E^-)}{(2\pi\hbar)^2}\,\{1 + O(\hbar)\}\ , \tag{5.3}
$$

where $\mathrm{vol}(\Omega_E^{\pm})$ denotes the volumes,

$$
\mathrm{vol}(\Omega_E^{\pm}) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \delta(H^{\pm}(\vec{p},\vec{x}) - E)\ \mathrm{d}^3p\,\mathrm{d}^3x\ , \tag{5.4}
$$

of the hypersurfaces $\Omega_E^{\pm}$.

For the computation of the contribution to (2.27) caused by the second class of stationary points, associated with the non-trivial classical periodic orbits, we proceed differently. As a starting point we consider the r.h.s. of (2.27), in which we introduce the semiclassical representation (3.27) of the truncated time evolution kernel. That is, we are going to evaluate

$$
\frac{1}{2\pi}\int_{\mathbb{R}^3}\int_{-\infty}^{+\infty} [1 - h(t)]\,\tilde{\varrho}(t)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}Et}\ \mathrm{tr}\,K_\chi(\vec{x},\vec{x},t)\ \mathrm{d}t\,\mathrm{d}^3x \tag{5.5}
$$

with the method of stationary phase, after having inserted the r.h.s. of (3.27) for $K_\chi(\vec{x},\vec{x},t)$. Notice that the factor $1 - h(t)$ cuts off a neighbourhood of $t = 0$ and that the compactly supported function $\tilde{\varrho}$ further restricts the range of integration over t to a bounded set. The semiclassical asymptotics (3.27), which was derived with t held fixed, can therefore be used in (5.5) without running into conflict with a need to perform $t \to \infty$. Apart from the factors caused by the spin degrees of freedom in (3.27), and from the fact that the two relativistic classical Hamiltonians $H^{\pm}(\vec{p},\vec{x})$ determine the equations of motion for the translational degrees of freedom, the following calculation is closely parallel to the case of the Schrödinger equation [10].

As implied by the discussion at the end of section 2, the stationary points relevant for the semiclassical evaluation of (5.5), which we now express as

$$\frac{1}{2\pi(2\pi \mathrm{i}\hbar)^{\frac{3}{2}}}\int_{\mathbb{R}^3}\int_{-\infty}^{+\infty}[1-h(t)]\,\tilde{\varrho}(t)\left\{\sum_{\gamma^+_{xx}}\chi(E_{\gamma^+_{xx}})\,\mathrm{tr}\left(V_t\,d_+\,V_0^\dagger\right)\,D^+_{\gamma^+_{xx}}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}[R^+_{\gamma^+_{xx}}+Et]-\mathrm{i}\frac{\pi}{2}\nu^+_{\gamma_{xx}}}+\right.$$
$$\left.\sum_{\gamma^-_{xx}}\chi(E_{\gamma^-_{xx}})\,\mathrm{tr}\left(W_t\,d_-\,W_0^\dagger\right)\,D^-_{\gamma^-_{xx}}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}[R^-_{\gamma^-_{xx}}+Et]-\mathrm{i}\frac{\pi}{2}\nu^-_{\gamma_{xx}}}\right\}\{1+O(\hbar)\}\,\mathrm{d}t\,\mathrm{d}^3x\ , \tag{5.6}$$

derive from the non-trivial periodic orbits $\gamma_p^\pm$. Indeed, the stationary points of the phases appearing in (5.6) are determined by

$$\left[\vec{\nabla}_{\vec{x}}R^\pm_{\gamma^\pm_{xy}}(\vec{x},\vec{y},t)+\vec{\nabla}_{\vec{y}}R^\pm_{\gamma^\pm_{xy}}(\vec{x},\vec{y},t)\right]_{\vec{y}=\vec{x}}=0 \quad \text{and} \quad -\frac{\partial R^\pm_{\gamma^\pm_{xx}}}{\partial t}(\vec{x},\vec{x},t)=E\ . \tag{5.7}$$

The first relation requires that initial and final momenta of those closed trajectories $\gamma^\pm_{xx}$ that contribute to the method of stationary phase must coincide, so that these are indeed periodic. The second condition then picks out those periodic orbits that are contained in the hypersurfaces $\Omega_E^\pm$. At stationary points the phases then read

$$R^\pm_{\gamma_p^\pm}(\vec{x}_{\gamma_p^\pm},\vec{x}_{\gamma_p^\pm},T_{\gamma_p^\pm})+E\,T_{\gamma_p^\pm}=\oint_{\gamma_p^\pm}\vec{p}\,\mathrm{d}\vec{x}=:S^\pm_{\gamma_p^\pm}(E)\ . \tag{5.8}$$

In order to apply the method of stationary phase to (5.6) we assume that all periodic orbits are isolated and non-degenerate. Strictly speaking, one now has to introduce a partition of unity that separates the contributions of the isolated orbits. Since their periods are known not to accumulate at some finite value T, this can be done in the same manner as for the trivial period $T_0=0$ above.

The only difference to the case of the Schrödinger equation is caused by the presence of the spin degrees of freedom. This is represented through the matrix trace under the integral in (5.6). At stationary points, however, $t=T_{\gamma_p^\pm}$ and the periodicity implies that $V_{T_{\gamma_p^+}}=V_0$. Thus a cyclic permutation under the matrix trace together with the former result (4.28) yields

$$\mathrm{tr}\big(V_{T_{\gamma_p^+}}\,d_{+,\gamma_p^+}\,V_0^\dagger\big)=\mathrm{tr}\big(V_0^\dagger\,V_0\,d_{+,\gamma_p^+}\big)=\mathrm{tr}\left(d_{+,\gamma_p^+}\right)=2\,\cos(\tfrac{1}{2}\theta_{\gamma_p^+})\,\cos\eta_{\gamma_p^+}\ . \tag{5.9}$$

Finishing the calculation as in the well known case of the Schrödinger equation [9, 10] finally yields a contribution of

$$\chi(E)\,\frac{\tilde{\varrho}(T_{\gamma_p^\pm})}{2\pi}\,A_{\gamma_p^\pm}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S_{\gamma_p^\pm}(E)}\,\{1+O(\hbar)\} \tag{5.10}$$

for every isolated non-degenerate periodic orbit $\gamma_p^\pm$. Here the amplitude $A_{\gamma_p^\pm}$ contains only classical information about the periodic orbit, including the contribution of a classical spin precessing along the orbit. Explicitly, the amplitude reads

$$A_{\gamma_p^\pm} = \frac{2\,T^\#_{\gamma_p^\pm}\,\cos(\frac{1}{2}\theta_{\gamma_p^\pm})\,\cos\eta_{\gamma_p^\pm}}{\left|\det(M_{\gamma_p^\pm} - \mathbb{1}_4)\right|^{1/2}}\,\mathrm{e}^{-\mathrm{i}\frac{\pi}{2}\mu_{\gamma_p^\pm}}\ . \tag{5.11}$$

In this expression $T^\#_{\gamma_p^\pm}$ denotes the primitive period of $\gamma_p^\pm$, i. e., the period of the associated primitive periodic orbit. Moreover, $M_{\gamma_p^\pm}$ is the linearised Poincaré map (monodromy matrix) along the orbit and $\mu_{\gamma_p^\pm}$ is its Maslov index.

From the Gutzwiller trace formula it is well known that if $\gamma_p^\pm$ is not primitive, all quantities that enter (5.10), apart from the spin contribution (5.9), can be readily expressed in terms of the respective quantities of the associated primitive periodic orbit. In order to extend this to (5.9) we recall that if $\gamma_p^\pm$ is a k-fold repetition of a primitive orbit, where $k \in \mathbb{Z}\setminus\{0\}$, the fact that d_{+,γ_p^+} is a holonomy implies that $d_{+,\gamma_p^+} = (d^\#_{+,\gamma_p^+})^k$, where $d^\#_{+,\gamma_p^+}$ denotes the corresponding primitive holonomy. According to [46] the trace (5.9) associated with $\gamma_p^\pm$ can hence be expressed as

$$\mathrm{tr}\big(d_{+,\gamma_p^+}\big) = T_k\left(\mathrm{tr}\big(d^\#_{+,\gamma_p^+}\big)\right)\ , \tag{5.12}$$

where $T_k(x)$ is the k-th Chebyshev polynomial of the second kind in x. Thus, if desired, the following trace formulae (5.13) and (5.15) can also be expressed in terms of sums over primitive periodic orbits and their repetitions.

In case the classical dynamics generated by the Hamiltonians $H^\pm$ have only isolated non-degenerate periodic orbits, the relations (5.3) and (5.10) now enable us to state the following semiclassical trace formula explicitly,

$$\begin{aligned}\sum_n \chi(E_n)\,\varrho\left(\frac{E_n - E}{\hbar}\right) &= \chi(E)\,\frac{\tilde{\varrho}(0)}{2\pi}\,\frac{2\,\mathrm{vol}\,(\Omega_E^+) + 2\,\mathrm{vol}\,(\Omega_E^-)}{(2\pi\hbar)^2}\,\{1 + O(\hbar)\}\\ &\quad + \sum_{\gamma_p^\pm} \chi(E)\,\frac{\tilde{\varrho}(T_{\gamma_p^\pm})}{2\pi}\,A_{\gamma_p^\pm}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S_{\gamma_p^\pm}(E)}\,\{1 + O(\hbar)\}\ .\end{aligned} \tag{5.13}$$

The conditions imposed on the test function ϱ and its Fourier transform ensure that all expressions entering this trace formula are finite. In particular, due to the compact support of $\tilde{\varrho}$ the sum over periodic orbits only includes orbits up to a finite period and since the Hamiltonian flow generated by $H^\pm(\vec{p},\vec{x})$ was supposed to be clean the sum is of finite length.

Often a semiclassical trace formula is presented for the spectral density of the quantum Hamiltonian, see e. g. [9, 10]. In the present case one can readily obtain such a trace formula for the truncated spectral density

$$d_\chi(E) := \sum_n \chi(E_n)\,\delta(E - E_n) \tag{5.14}$$

from (5.13). This reads

$$d_\chi(E) = \chi(E)\,\frac{2\,\mathrm{vol}(\Omega_E^+) + 2\,\mathrm{vol}(\Omega_E^-)}{(2\pi\hbar)^3}\,\{1+O(\hbar)\}$$
$$+\,\chi(E)\,\frac{1}{\pi\hbar}\sum_{\gamma_p^\pm}\frac{T^\#_{\gamma_p^\pm}\cos(\frac{1}{2}\theta_{\gamma_p^\pm})\cos\eta_{\gamma_p^\pm}}{\left|\det(M_{\gamma_p^\pm}-\mathbb{1}_4)\right|^{1/2}}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S_{\gamma_p^\pm}(E)-\mathrm{i}\frac{\pi}{2}\mu_{\gamma_p^\pm}}\,\{1+O(\hbar)\}\ . \tag{5.15}$$

Obviously, the sum over classical periodic orbits in (5.15) does not converge. This trace formula rather has to be viewed as a distributional identity whose actual meaning is provided by (5.13).

6 Nonrelativistic limit

As compared to the Schrödinger equation, the Dirac equation takes two generalisations into account. It first takes care of the spin degrees of freedom and, secondly, describes relativistic dynamics. In many situations of physical interest it, however, suffices only to include spin and to leave the description of the translational motion on a nonrelativistic level. As it is well known, this can be achieved by considering the Pauli equation, possibly with several additional terms such as one describing spin-orbit coupling. In this section we therefore want to study particles of charge e and mass m with spin 1/2 in a nonrelativistic context. To this end we compare the semiclassical asymptotics for the Pauli equation with the leading order as $c\to\infty$ of the time evolution kernel (3.27) for the Dirac equation. Both approaches, which will turn out to produce identical results, then allow to set up a semiclassical trace formula.

We recall that when one divides a Dirac four-spinor Ψ into two-spinors $\psi_{1/2}$ according to

$$\Psi(\vec{x},t) =: \begin{pmatrix}\psi_1(\vec{x},t)\\ \psi_2(\vec{x},t)\end{pmatrix}\ , \tag{6.1}$$

one obtains from (2.1) two coupled matrix differential equations. It is well known [36] that to leading order as $c\to\infty$ these equations decouple, and that for $\psi:=\psi_1$ the Pauli equation

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t}(\vec{x},t) = \left[\frac{1}{2m}\left(\frac{\hbar}{\mathrm{i}}\vec{\nabla}_{\vec{x}}-\frac{e}{c}\vec{A}(\vec{x})\right)^2 + e\,\varphi(\vec{x}) - \frac{e\hbar}{2mc}\,\vec{\sigma}\vec{B}(\vec{x})\right]\psi(\vec{x},t) =: \hat{H}_P\psi(\vec{x},t) \tag{6.2}$$

emerges. See also [38] for a careful treatment of the limit $c\to\infty$. In Weyl quantisation the Pauli Hamiltonian $\hat{H}_P$ can be realised as

$$\hat{H}_P = H_P\left(\frac{\hbar}{\mathrm{i}}\vec{\nabla}_{\vec{x}},\vec{x}\right)\ , \tag{6.3}$$

with the 2×2 symbol matrix

$$H_P(\vec{p}, \vec{x}) = H_0(\vec{p}, \vec{x}) + \hbar\, H_1(\vec{p}, \vec{x}) \ . \tag{6.4}$$

As opposed to the Dirac equation, compare (2.5), this Weyl symbol is composed of a principal symbol

$$H_0(\vec{p}, \vec{x}) := \left[\frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}(\vec{x})\right)^2 + e\,\varphi(\vec{x})\right]\mathbb{1}_2 \ , \tag{6.5}$$

which is a multiple of the identity matrix, and an additional subprincipal symbol

$$H_1(\vec{p}, \vec{x}) = -\frac{e}{2mc}\,\vec{\sigma}\vec{B}(\vec{x}) \tag{6.6}$$

that reflects a coupling of the spin degrees of freedom to the external magnetic field.

We are now going to study the semiclassical limit $\hbar \to 0$ along the lines developed above for the Dirac equation. Since therefore many details of the following calculations are similar to the ones shown in the previous sections, at several places the presentation will be kept rather brief. The matrix-valued Schwartz kernel $K_P(\vec{x}, \vec{y}, t)$ of the time evolution operator $\hat{U}_P(t) := \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_P t}$ obeys

$$\psi(\vec{x}, t) = \int_{\mathbb{R}^3} K_P(\vec{x}, \vec{y}, t)\,\psi_0(\vec{y})\,\mathrm{d}^3 y \ , \quad \psi(\vec{x}, 0) = \psi_0(\vec{x}) \ , \tag{6.7}$$

so that $K_P(\vec{x}, \vec{y}, t)$ has to solve the Pauli equation (6.2) with initial condition

$$\lim_{t \to 0+} K_P(\vec{x}, \vec{y}, t) = \mathbb{1}_2\,\delta(\vec{x} - \vec{y}) \ . \tag{6.8}$$

Since the principal symbol H_0 is a scalar multiple of the identity matrix and thus has one eigenvalue, only one Hamilton-Jacobi equation will be relevant to the semiclassical time evolution. We therefore choose the semiclassical ansatz

$$K_P(\vec{x}, \vec{y}, t) = \frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^3}\left[\sum_{k=0}^{\infty}\left(\frac{\hbar}{\mathrm{i}}\right)^k a_k(\vec{x}, \vec{y}, t; \vec{\xi})\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S(\vec{x}, \vec{\xi}, t) - \vec{y}\vec{\xi})}\right]\mathrm{d}^3\xi + O(\hbar^\infty) \ , \tag{6.9}$$

compare (2.8) and (2.14), which we introduce into (6.2). Comparing like orders in $\hbar$ yields to lowest order a Hamilton-Jacobi equation for S, whereas to orders $\hbar^k$, $k = 1, 2, 3, \ldots$, transport equations for the 2×2 matrices a_{k-1} follow. The initial conditions for $S - \vec{y}\vec{\xi}$ and a_k are analogous to (2.10) and (2.11). By obvious reasons, the subprincipal symbol (6.6) cannot appear to zeroth order in $\hbar$ so that the Hamilton-Jacobi equation emerging in leading semiclassical order is only determined by the principal symbol $H_0(\vec{p}, \vec{x})$. As a consequence, the classical dynamics of the translational degrees of freedom are those of a nonrelativistic point particle that does not experience a force coming from a coupling of spin to the external magnetic field. The latter is, however, contained in the transport equation for a_0 that appears in next-to-leading order. This reads

$$\left[\vec{\nabla}_{\vec{p}}H_0(\vec{\nabla}_{\vec{x}}S,\vec{x})\vec{\nabla}_{\vec{x}}+\frac{\partial}{\partial t}+\frac{1}{2}\vec{\nabla}_{\vec{x}}\left[\vec{\nabla}_{\vec{p}}H_0(\vec{\nabla}_{\vec{x}}S,\vec{x})\right]+\mathrm{i}M_P(\vec{x})\right]a_0=0\ , \tag{6.10}$$

so that the spin degrees of freedom enter through the traceless hermitian 2×2 matrix

$$M_P(\vec{x}):=-\frac{e}{2mc}\vec{\sigma}\vec{B}(\vec{x})\equiv H_1(\vec{\nabla}_{\vec{x}}S,\vec{x})\ . \tag{6.11}$$

In analogy to the considerations following (3.14), the ansatz

$$a_0(\vec{X}(t),\vec{y},t;\vec{\xi}_j)=\sqrt{\det\left(\frac{\partial^2 S}{\partial x_k\partial\xi_l}(\vec{x},\vec{\xi}_j,t)\right)}\,d_P(\vec{P}(t),\vec{X}(t))\ , \tag{6.12}$$

for the lowest order amplitude, evaluated along a classical trajectory γ_{xy} associated with the stationary point $\vec{\xi}_j$ of the phase, proves useful. It leads to the nonrelativistic spin transport equation

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}+\mathrm{i}M_P(\vec{X}(t))\right]d_P(\vec{P}(t),\vec{X}(t))=0\ ,\quad d_P(\vec{P}(0),\vec{X}(0))=\mathbb{1}_2\ , \tag{6.13}$$

along γ_{xy} that determines the SU(2) matrix $d_{P,\gamma_{xy}}$ describing the leading contribution of spin to the semiclassical time evolution kernel. The transport equations (6.10) and (6.13) have already been obtained by Choquard [47], who used a semiclassical ansatz similar to (6.9), however, without the integration over $\vec{\xi}$.

We remark that the decomposition of the SU(2) matrix d_+ into a classical spin $\vec{s}$ and an additional phase η presented in section 4 can be repeated in the present, nonrelativistic, context. This procedure leads to the dynamical equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{s}=\vec{s}\times\frac{e}{mc}\vec{B} \tag{6.14}$$

for $\vec{s}$ transported along γ_{xy} in the external magnetic field. The r.h.s. of (6.14) can readily be identified as the leading order of the r.h.s. of (4.17) as $c\to\infty$. An additional phase,

$$\eta_P(t)=\frac{e}{2mc}\int_0^t\vec{B}(t')\vec{s}(t')\ \mathrm{d}t'-\frac{1}{2}\int_0^t\big(1-\cos\theta(t')\big)\frac{\mathrm{d}\phi}{\mathrm{d}t'}(t')\ \mathrm{d}t'\ , \tag{6.15}$$

representing the third, nonclassical, degree of freedom of d_P, appears in the same manner as for the Dirac equation. This phase is again composed of a dynamical and a geometric part.

A calculation similar to that presented in section 3 finally leads to the following semiclassical time evolution kernel for the Pauli equation (for $t\neq 0$),

$$K_P(\vec{x},\vec{y},t)=\frac{1}{(2\pi\mathrm{i}\hbar)^{3/2}}\sum_{\gamma_{xy}}d_{P,\gamma_{xy}}\,D_{\gamma_{xy}}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}R_{\gamma_{xy}}-\mathrm{i}\frac{\pi}{2}\nu_{\gamma_{xy}}}\{1+O(\hbar)\}\ . \tag{6.16}$$

On the r.h.s. the sum extends over the solutions of Hamilton's equations of motion with the classical Hamiltonian $H_0(\vec{p},\vec{x})$, which connect $\vec{y}$ and $\vec{x}$ in time t. The corresponding Morse indices and Hamilton's principal functions are denoted by $\nu_{\gamma_{xy}}$ and $R_{\gamma_{xy}}(\vec{x},\vec{y},t)$, respectively; compare (3.18). The factor $D_{\gamma_{xy}}$ is defined by

$$D_{\gamma_{xy}} := \left| \det \left(-\frac{\partial^2 R_{\gamma_{xy}}}{\partial x_k \partial y_l}(\vec{x},\vec{y},t) \right) \right|^{1/2} . \tag{6.17}$$

Since these quantities are already determined by the nonrelativistic classical dynamics generated by H_0, the only difference between (6.16) and the respective semiclassical kernel for the Schrödinger equation is an appearence of the factors $d_{P,\gamma_{xy}} \in \mathrm{SU}(2)$ that represent the leading influence of spin.

So far we have examined the propagator that emerges from first taking the nonrelativistic limit of the Dirac equation and then constructing a semiclassical time evolution kernel. We will now compare this to the result that one obtains by first constructing the relativistic semiclassical kernel (3.27) and then taking the nonrelativistic limit. We are thus now interested in the leading order behaviour of (3.27) as $c \to \infty$. To this end we first remark that

$$V(\vec{p},\vec{x}) = \begin{pmatrix} \mathbb{1}_2 \\ 0 \end{pmatrix} + O\left(\tfrac{1}{c}\right) , \quad W(\vec{p},\vec{x}) = \begin{pmatrix} 0 \\ \mathbb{1}_2 \end{pmatrix} + O\left(\tfrac{1}{c}\right) , \quad c \to \infty , \tag{6.18}$$

i. e., in leading order the positive and negative kinetic energy parts in (3.27) decouple completely. We therefore have to compare (6.16) with the upper left 2×2 block of (3.27). This is consistent with (6.1) because this block describes the time evolution of the two-spinor $\psi = \psi_1$. We furthermore recall the well known fact that the classical relativistic dynamics described by $H^+(\vec{p},\vec{x})$ turns into the nonrelativistic dynamics with the classical Hamiltonian $H_0(\vec{p},\vec{x})$ as $c \to \infty$. This in particular implies that γ^+_{xy}, $R^+_{\gamma^+_{xy}}$, $\nu^+_{\gamma^+_{xy}}$ and $D^+_{\gamma^+_{xy}}$ may in leading order be approximated by γ_{xy}, $R_{\gamma_{xy}}$, $\nu_{\gamma_{xy}}$ and $D_{\gamma_{xy}}$. We are therefore only left with comparing the factors d_+ and d_P which describe the influence of spin in a relativistic and in a nonrelativistic context, respectively. As already mentioned below equation (6.14)

$$M_+ = M_P + O(\tfrac{1}{c}) , \quad c \to \infty , \tag{6.19}$$

leads to a nonrelativistic approximation for both the classical spin dynamics and the non-classical phase. Thus d_P provides the leading order asymptotical term for d_+ as $c \to \infty$. Collecting everything one observes that in the nonrelativistic limit the upper left block of the semiclassical time evolution kernel (3.27) for the Dirac equation turns into the respective result (6.16) for the Pauli equation. In this sense the limits $\hbar \to 0$ and $c \to \infty$ commute, at least concerning leading orders.

In order to set up a semiclassical trace formula for the Pauli Hamiltonian we now assume that $\hat{H}_P$ has a pure point spectrum. Otherwise we would have to employ an energy localisation to a gap in the essential spectrum as described in section 2 for the

Dirac Hamiltonian. We then consider a test function $\varrho \in \mathcal{S}(\mathbb{R})$ with compactly supported Fourier transform $\tilde{\varrho}$. Applying the procedure of section 5 to $\hat{H}_P$ finally yields

$$\begin{aligned}\sum_n \varrho\left(\frac{E_n - E}{\hbar}\right) &= \frac{\tilde{\varrho}(0)}{2\pi}\,\frac{2\,\mathrm{vol}(\Omega_E)}{(2\pi\hbar)^2}\,\{1 + O(\hbar)\} \\ &\quad + \sum_{\gamma_p} \frac{\tilde{\varrho}(T_{\gamma_p})}{2\pi}\,A_{\gamma_p}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S_{\gamma_p}(E)}\,\{1 + O(\hbar)\}\ ,\end{aligned} \tag{6.20}$$

where the sum extends over the periodic orbits of the classical dynamics generated by the principal symbol H_0. In fact, all classical quantities entering (6.20) refer to this Hamiltonian. As explained in the relativistic case, for such a trace formula to be valid the flow generated by H_0 must be clean. The amplitude associated with each isolated, non-degenerate periodic orbit then reads

$$A_{\gamma_p} = \frac{2\,T^{\#}_{\gamma_p}\,\cos(\frac{1}{2}\theta_{\gamma_p})\,\cos\eta_{P,\gamma_p}}{\left|\det(M_{\gamma_p} - \mathbb{1}_4)\right|^{1/2}}\,\mathrm{e}^{-\mathrm{i}\frac{\pi}{2}\mu_{\gamma_p}}\ . \tag{6.21}$$

A different semiclassical approach to the Pauli equation has previously been used to investigate spin-orbit coupling [33, 34]. The authors of these papers principally base their method on the technique developed by Littlejohn and Flynn [6, 7] to treat matrix-valued wave operators with principal symbols that have no (globally) degenerate eigenvalues. Below we will derive the time evolution according to the prescription of the semiclassical limit employed in [33, 34], however, using the techniques outlined in the previous sections. For simplicity, and for ease of comparison with our previous semiclassical study of the Pauli equation, we will not consider spin-orbit coupling but only a coupling of spin to the external magnetic field. Therefore, the relevant Hamiltonian is the one defined in (6.2). However, a generalisation of the following discussion to arbitrary couplings of the form $\vec{\sigma}\,\vec{C}(\vec{p},\vec{x})$ is straight forward. Following now the philosophy of [33, 34], we introduce Bohr's magneton $\mu := \frac{e\hbar}{2mc}$ and consider it as constant in the semiclassical limit. Thus the Hamiltonian

$$\hat{H}'_P := \frac{1}{2m}\left(\frac{\hbar}{\mathrm{i}}\vec{\nabla} - \frac{e}{c}\vec{A}(\vec{x})\right)^2 + e\,\varphi(\vec{x}) - \mu\,\vec{\sigma}\vec{B}(\vec{x}) \tag{6.22}$$

arises as a Weyl operator associated with the symbol

$$H'_P(\vec{p},\vec{x}) := \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}(\vec{x})\right)^2 + e\,\varphi(\vec{x}) - \mu\,\vec{\sigma}\vec{B}(\vec{x})\ , \tag{6.23}$$

so that no subprincipal symbol occurs. As opposed to the situation analysed at the beginning of this section, one could view the present procedure as taking the simultaneous limits $\hbar \to 0$ and $|\vec{B}| \to \infty$ in such a way that $\hbar|\vec{B}| = const.$ Another way to look at this is to keep $|\vec{B}|$ fixed, but to perform the limit of 'large spin'.

As long as $\vec{B} \neq 0$ the 2×2 symbol matrix (6.23) has two non-degenerate eigenvalues

$$H'^{\pm}_P(\vec{p},\vec{x}) = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}(\vec{x})\right)^2 + e\,\varphi(\vec{x}) \mp \mu\,|\vec{B}(\vec{x})|\ , \tag{6.24}$$

which generate two classes of classical dynamics. Since this is similar to the situation occurring for the Dirac equation, the semiclassical ansatz for the time evolution kernel $K'_P(\vec{x},\vec{y},t)$ therefore should be chosen as in (2.8), but where now the amplitudes are 2×2 matrices. Applying the procedure described in section 3 then leads to two Hamilton-Jacobi equations, with the two Hamiltonians (6.24).

The non-scalar contribution to the symbol matrix (6.23) is given by the Hamiltonian $-\mu\,\vec{\sigma}\vec{B}(\vec{x})$ describing a quantum mechanical precessing spin. The orthonormal eigenvectors $v_\pm(\vec{x})\in\mathbb{C}^2$ of $H'_P(\vec{p},\vec{x})$ corresponding to the eigenvalues $H'^{\pm}_P(\vec{p},\vec{x})$ are hence well known from the standard example of the Berry phase [29]. In analogy to (3.5) one can now introduce the ansatz

$$a_0^+(\vec{x},\vec{y},t;\vec{\xi}) = v_+(\vec{x})\,\tilde{v}^\dagger(\vec{x},\vec{\xi},t) \tag{6.25}$$

with some suitable vector $\tilde{v}\in\mathbb{C}^2$. Upon multiplication of the transport equation for a_0^+ with $v_+^\dagger(\vec{x})$ from the left one obtains the equation

$$\left[\vec{\nabla}_{\vec{p}}H'^{+}_P(\vec{\nabla}_{\vec{x}}S^+,\vec{x})\vec{\nabla}_{\vec{x}} + \frac{\partial}{\partial t} + \frac{1}{2}\vec{\nabla}_{\vec{x}}\left[\vec{\nabla}_{\vec{p}}H'^{+}_P(\vec{\nabla}_{\vec{x}}S^+,\vec{x})\right] + \mathrm{i}M'^{+}_P(\vec{\nabla}_{\vec{x}}S^+,\vec{x})\right]\tilde{v}^\dagger = 0\ , \tag{6.26}$$

where

$$M'^{+}_P(\vec{p},\vec{x}) := -\frac{\mathrm{i}}{m}\left(\vec{p}-\frac{e}{c}\vec{A}(\vec{x})\right)\,v_+^\dagger(\vec{x})\vec{\nabla}_{\vec{x}}v_+(\vec{x})\ . \tag{6.27}$$

On the r.h.s., the factor $v_+^\dagger\vec{\nabla}v_+$ is the well known expression for the adiabatic connection leading to the U(1)-Berry phase of a precessing spin [29]. Again, the transport equations for $a_0^\pm$ will be solved along the classical trajectories $\gamma'^{\pm}_{xy}$ following from the Hamiltonians (6.24). As suggested by (3.15) and (3.20), one separates

$$\tilde{v}^\dagger(\vec{X}(t),\vec{\xi}_j,t) = \sqrt{\det\left(\frac{\partial^2 S^+}{\partial x_k\partial\xi_l}(\vec{X}(t),\vec{\xi}_j,t)\right)}\;d'_+(\vec{P}(t),\vec{X}(t))\;v_+^\dagger(\vec{y})\ , \tag{6.28}$$

so that along a trajectory γ'^{+}_{xy} the phase $d'_+(t)\in\mathrm{U}(1)$ has to solve the equation

$$\left[\frac{\mathrm{d}}{\mathrm{d}t} + v_+^\dagger(\vec{X}(t))\vec{\nabla}_{\vec{x}}v_+(\vec{X}(t))\,\dot{\vec{X}}(t)\right]d'_+(t) = 0\ ,\qquad d'_+(0)=1\ . \tag{6.29}$$

As a result, one obtains the well known U(1)-Berry phase of a quantum mechanical spin that has been transported adiabatically along the trajectory γ'^{+}_{xy}. Finally, the semiclassical time evolution kernel reads

$$K'_P(\vec{x},\vec{y},t) = \frac{1}{(2\pi\mathrm{i}\hbar)^{3/2}}\sum_{\gamma'^{\pm}_{xy}} v_\pm(\vec{x})v_\pm^\dagger(\vec{y})\,d'_\pm\,D^{\pm}_{\gamma'^{\pm}_{xy}}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}R'^{\pm}_{\gamma'^{\pm}_{xy}}-\mathrm{i}\frac{\pi}{2}\nu_{\gamma'^{\pm}_{xy}}}\,\{1+O(\hbar)\}\ , \tag{6.30}$$

where all classical quantities refer to the dynamics generated by the Hamiltonians (6.24) and are defined in analogy to the previous cases. In particular, Hamilton's principal functions $R'^{\pm}_{\gamma'^{\pm}_{xy}}(\vec{x},\vec{y},t)$ are related to the analogous quantities $R_{\gamma'^{\pm}_{xy}}(\vec{x},\vec{y},t)$ that are defined by the Hamiltonian (6.5), but here evaluated along the trajectories $\gamma'^{\pm}_{xy}$, through

$$R'^{\pm}_{\gamma'^{\pm}_{xy}}(\vec{x},\vec{y},t) = R_{\gamma'^{\pm}_{xy}}(\vec{x},\vec{y},t) \pm \mu \int_0^t |\vec{B}(\vec{X}(t'))| \, \mathrm{d}t' \; . \tag{6.31}$$

Due to the factors $v_{\pm}(\vec{x})v^{\dagger}_{\pm}(\vec{y})$ in (6.30) the 'spin up' and 'spin down' components of an initial spinor $\psi_0(\vec{y})$ are propagated independently along the corresponding trajectories following from the Hamiltonians $H'^{\pm}_{P}$. Here 'spin up' and 'spin down' are defined with respect to the instantaneous direction of the magnetic field. This procedure breaks down at mode conversion points, i. e., at points where the magnetic field vanishes. There the symbol matrix (6.23) has one twofold degenerate eigenvalue and the level surfaces of the two Hamiltonians $H'^{\pm}_{P}$ cross. Moreover, since $\vec{\nabla}_{\vec{x}} H'^{\pm}_{P}$ develops a singularity, the classical trajectories are not smooth when crossing a mode conversion point. In certain situations this defect can be cured by letting the trajectories cross the two level surfaces, see [34], but in general an application of the present semiclassical procedure requires a more refined treatment of mode conversion points, see [48] for a detailed discussion.

At this place one could easily establish the corresponding semiclassical trace formula, if one followed the programme outlined in section 2 once again. However, we refrain from doing this here and rather comment on the relation between the two semiclassical approaches to the Pauli equation discussed in this chapter, which lead to the two distinct expressions (6.16) and (6.30) for the time evolution kernel. In the first scenario we systematically performed an expansion in $\hbar$ and determined the leading order terms for the time evolution kernel and for the classical side of the trace formula. We observed that to lowest order the translational degrees of freedom decouple from the spin degrees of freedom in that the translational motion experiences no back reaction from the coupling of spin to the external magnetic field. In a certain sense this decoupling can be seen as an adiabatic one where the translational motion is considered as slow, although this condition is not needed for the formulae to be valid. This topic was also discussed by Balian and Bloch [24] in the context of semiclassical approximations for the Green function. Spin enters in next-to-leading order and, among other quantities, determines the amplitudes in the relevant semiclassical expressions. The leading order of the spin dynamics is given by that of a classical spin precessing along the particle trajectories. We have repeatedly emphasized that at this stage no adiabatic limit is considered. In addition, a geometric phase of the type discussed by Aharonov and Anandan [32] enters the amplitudes. In the second scenario we considered the double limit $\hbar \to 0$, $|\vec{B}| \to \infty$, $\hbar|\vec{B}| = const.$ It turned out that in this context the relevant classical translational motion follows from two Hamiltonians, taking the effect of a coupling of a 'spin up' and a 'spin down', respectively, to the external magnetic field into account. Since in this context, via the expressions $v_{\pm}(\vec{x})v^{\dagger}_{\pm}(\vec{y})$ in (6.30), the spin direction is defined with respect to the instantaneous direction of the magnetic field, the spin degrees of freedom are transported adiabatically along the particle trajectories. There is no further dynamical equation for a classical spin and, as a consequence of the limit $|\vec{B}| \to \infty$, the Berry phase that enters can be viewed as emerging from an adiabatic approximation of the geometric term found in the first scenario. This finding is in agreement with the remark on the relation of these phases that can be found in [32]. In order to be more specific concerning the issue of adiabaticity, we introduce spherical coordinates (ϑ_B, φ_B) for $\vec{B}/|\vec{B}|$ which allows to obtain an explicit expression for the Berry phase emerging from (6.29). Moreover, we reintroduce $\frac{e\hbar}{2mc}$ for the magneton μ. Using (6.31) one thus observes that

$$d'_{\pm}\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar} R'^{\pm}_{\gamma'^{\pm}_{xy}}} = \exp\left\{ \pm \mathrm{i} \frac{e}{2mc} \int_0^t |\vec{B}|\, \mathrm{d}t' \mp \frac{\mathrm{i}}{2} \int_0^t (1-\cos\vartheta_B)\, \dot{\varphi}_B\, \mathrm{d}t' \right\}\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar} R_{\gamma'^{\pm}_{xy}}}\,, \tag{6.32}$$

which can be introduced in (6.30). The first factor on the r.h.s. is readily identified to arise as an adiabatic approximation to $\mathrm{e}^{\pm \mathrm{i}\eta_P}$, if the phase (6.15) is evaluated along the trajectory γ'^{+}_{xy} instead of γ_{xy}. Thus the spin contributions to (6.30) are adiabatic approximations to the respective contributions to (6.16). Conversely, one concludes that in the semiclassical time evolution according to (6.16) the spin transport is performed non-adiabatically so that mode conversion poses no difficulty. In conclusion, one can consider the two alternative ways of performing the semiclassical limit as being considered with a 'weak' and a 'strong' coupling, respectively, of spin to the translational degrees of freedom. Comparing the two results (6.16) and (6.30) for the time evolution kernel one notices that the two approaches yield different results when extended to intermediate couplings. In the first case the translational motion is not influenced by the spin, whose dynamics in turn is not treated adiabatically. In the second case, however, spin has an effect on the translational motion, but the spin dynamics enters in an adiabatic approximation. This observation illustrates the fact that the $\hbar$-expansions employed are not uniform in the field strength.

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