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Semiclassical Time Evolution and Trace Formula for Relativistic Spin-1/2 Particles

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We investigate the Dirac equation in the semiclassical limit $\hbar \rightarrow 0$. A semiclassical propagator and a trace formula are derived and are shown to be determined by the classical orbits of a relativistic point particle. In addition, two phase factors enter, one of which can be calculated from the Thomas precession of a classical spin transported along the particle orbits. For the second factor we provide an interpretation in terms of dynamical and geometric phases. [S0031-9007(98)07032-X]

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The first one to seek a semiclassical treatment of the Dirac equation in the spirit of the WKB method appears to be Pauli [1], who gave a solution for a special case. He found that in the semiclassical limit the translational motion is independent of the spin degrees of freedom. Because of this fact the formalism was criticized by de Broglie [2] with the remark that one would expect “classical objects” like electromagnetic moments to influence the trajectories. This controversy was clarified by Rubinow and Keller [3] in a paper that seems to have been overlooked by some later authors. Rubinow and Keller pointed out that the moments of an electron are proportional to \hbar so that in leading order as $\hbar \rightarrow 0$ the influence of spin on the trajectories vanishes. However, in next-to-leading order the dynamical equation for Thomas precession [4] is obtained from the Dirac equation. Since only the ratio of the magnetic moment and spin enters this equation, it contains no \hbar and therefore can be interpreted as describing the dynamics of a classical spin.

The general setup for semiclassical quantization in the case of multicomponent wave equations was developed by Littlejohn and Flynn [5]. In a short-wavelength approximation they replaced the matrix-valued wave operator by a matrix-valued Hamiltonian function, such that its eigenvalues generate Hamiltonian dynamics in phase space. But even if these are integrable, an application of Einstein-Brillouin-Keller (EBK) quantization was found to be obstructed by the presence of additional phases. In [5] a formalism was presented that allows one to treat

matrix Hamiltonians with no (globally) degenerate eigenvalues. Subsequently, Emmrich and Weinstein [6] outlined how to proceed in the degenerate case that, e.g., occurs for the Dirac equation, and pointed out the problems of formulating a Bohr-Sommerfeld quantization. They, moreover, uncovered the global geometric meaning of the additional phases. A semiclassical quantization for special configurations, based on the complex WKB method, is presented in [7]. Based on the method developed in [5], the effect of spin-orbit coupling, which follows from the Dirac equation, is investigated semiclassically in a nonrelativistic context in [8].

In this paper we will follow an alternative approach in that we investigate the semiclassical time evolution and then set up a trace formula. This procedure avoids (some) difficulties that one encounters with semiclassical approximations to eigenspinors and, furthermore, is not restricted to classically integrable systems. We basically follow the approach that was developed by Gutzwiller [9] for the Schrödinger equation. Hence the basic object to be studied is the integral kernel $K(\mathbf{x}, \mathbf{y}, t)$ of the time evolution operator $U(t)$. Gutzwiller represented the kernel by a path integral and evaluated this semiclassically. However, here we prefer to use a representation of the kernel in terms of an oscillatory integral. This procedure can be made mathematically rigorous as, e.g., explained in [10] for the Schrödinger equation. In a second step we pass to the energy domain via Fourier transform, and then take the trace over spatial coordinates as well as over spin degrees of

freedom. This results in a periodic orbit formula for spectral functions. Special attention is paid to the role of spin. Our philosophy of a systematic semiclassical expansion in the context of the Dirac equation automatically ensures that spin is treated quantum mechanically from the outset, without any *ad hoc* semiclassical approximation. As mentioned above, the semiclassical asymptotics introduces an adiabatic decoupling of (slow) translational and (fast) spin degrees of freedom. This happens in such a way that to lowest orders in \hbar the expected dynamical equations for both kinds of degrees of freedom emerge. In addition, our procedure allows one to reinterpret the additional phases in terms of dynamical and geometric phases associated with a precessing spin. The degree of freedom that is lost upon passing from a quantum mechanical description of spin in terms of SU(2) matrices to a classical description in terms of vectors $\mathbf{s} \in \mathbb{R}^3$ with fixed length $|\mathbf{s}|$ can be reconstructed from one of these phases. A detailed account of our approach will be presented elsewhere [11].

Let us now briefly summarize the calculations and results. We investigate the Dirac equation

$$i\hbar \frac{\partial \Psi(\mathbf{x}, t)}{\partial t} = H_D \Psi(\mathbf{x}, t) \quad (1)$$

with the (quantum) Hamiltonian

$$H_D := c \boldsymbol{\alpha} \cdot \left[\frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A}(\mathbf{x}) \right] + \beta mc^2 + e \varphi(\mathbf{x}) \quad (2)$$

that acts on a suitable domain in the Hilbert space $L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$. The Dirac algebra is realized by

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} \mathbb{1}_{2 \times 2} & 0 \\ 0 & -\mathbb{1}_{2 \times 2} \end{pmatrix}, \quad (3)$$

where $\boldsymbol{\sigma}$ is the vector of Pauli matrices. The time evolution kernel is defined by

$$\Psi(\mathbf{x}, t) = \int_{\mathbb{R}^3} K(\mathbf{x}, \mathbf{y}, t) \Psi_0(\mathbf{y}) d^3 y \quad (4)$$

so that it has to fulfill the Dirac equation for $t > 0$ with initial condition $K(\mathbf{x}, \mathbf{y}, 0) = \mathbb{1}_{4 \times 4} \delta(\mathbf{x} - \mathbf{y})$. Anticipating the occurrence of solutions of appropriate classical equations of motion for positive and negative energies, respectively, we choose the semiclassical ansatz

$$K(\mathbf{x}, \mathbf{y}, t) = \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^3} [a_{\hbar}^+ e^{(i/\hbar)\phi^+} + a_{\hbar}^- e^{(i/\hbar)\phi^-}] d^3 \xi \quad (5)$$

with phase functions $\phi^{\pm} = \phi^{\pm}(\mathbf{x}, \mathbf{y}, t; \boldsymbol{\xi})$. The amplitudes a_{\hbar}^{\pm} are 4×4 matrices with semiclassical expansions

$$a_{\hbar}^{\pm}(\mathbf{x}, \mathbf{y}, t; \boldsymbol{\xi}) = \sum_{k=0}^{\infty} (-i\hbar)^k a_k^{\pm}(\mathbf{x}, \mathbf{y}, t; \boldsymbol{\xi}). \quad (6)$$

In order to account for the initial condition of the kernel, we have to choose $\phi^{\pm}|_{t=0} = (\mathbf{x} - \mathbf{y}) \cdot \boldsymbol{\xi}$ and

$a_{\hbar}^+|_{t=0} + a_{\hbar}^-|_{t=0} = \mathbb{1}_{4 \times 4}$. Inserting (5) into (1) and comparing like orders in \hbar yields to lowest order matrix equations which have solutions with nonzero a_0^{\pm} only if ϕ^{\pm} satisfy the Hamilton-Jacobi equations

$$H^{\pm}(\nabla_x \phi^{\pm}, \mathbf{x}) + \frac{\partial \phi^{\pm}}{\partial t} = 0 \quad (7)$$

with the (classical) Hamiltonians

$$H^{\pm}(\mathbf{p}, \mathbf{x}) = e\varphi(\mathbf{x}) \pm \sqrt{c^2 \left(\mathbf{p} - \frac{e}{c} \mathbf{A}(\mathbf{x}) \right)^2 + m^2 c^4}. \quad (8)$$

These are the (twofold degenerate) eigenvalues of the matrix-valued symbol $c \boldsymbol{\alpha} \cdot (\mathbf{p} - e/c \mathbf{A}) + \beta mc^2 + e\varphi$ of H_D . Because of (7) one can separate \mathbf{y} in ϕ^{\pm} according to $\phi^{\pm} = S^{\pm}(\mathbf{x}, \boldsymbol{\xi}, t) - \mathbf{y} \cdot \boldsymbol{\xi}$. When one applies the method of stationary phase to (5) as $\hbar \rightarrow 0$, it turns out that at stationary points S^{\pm} generates a canonical transformation that describes the dynamics of a relativistic point particle from \mathbf{y} to \mathbf{x} in time t .

We now turn to the equations that occur in next-to-leading order in \hbar , and which contain terms involving both a_0^+ and a_1^+ . Here we restrict to the index $+$. An equation for a_0^+ only is obtained through a multiplication on the left with the Hermitian conjugate V_t^{\dagger} of the 4×2 -matrix

$$V_t := V(\mathbf{x}, \mathbf{y}, t; \boldsymbol{\xi}) = \frac{1}{\sqrt{2\epsilon(\epsilon + mc^2)}} \begin{pmatrix} \epsilon + mc^2 \\ c \boldsymbol{\sigma} \cdot \boldsymbol{\pi} \end{pmatrix} \quad (9)$$

with $\epsilon := \sqrt{c^2 \boldsymbol{\pi}^2 + m^2 c^4}$ and $\boldsymbol{\pi} = \nabla_x \phi - \frac{e}{c} \mathbf{A}$, whose columns are the eigenvectors associated with H^+ . (We will denote by W_t the corresponding matrix of eigenvectors associated with H^- .) We then define a 2×2 matrix b_+ by

$$a_0^+ = V_t b_+ V_0^{\dagger} \quad (10)$$

and remark that only this construction with V_t on the left, together with the appropriate ϕ^+ , ensures that the equation to *lowest* order in \hbar is fulfilled. Moreover, at $t = 0$ the initial condition $b_+|_{t=0} = \mathbb{1}_{2 \times 2}$ ensures that $a_0^+|_{t=0} = V_0 V_0^{\dagger}$ is the projector on the H^+ eigenspace. A respective remark applies to a_0^- so that the initial condition for $a_0^+ + a_0^-$ is fulfilled. An obvious interpretation of this ansatz is as follows. Given an initial 4-spinor Ψ_0 at time $t = 0$, V_0^{\dagger} projects it onto the H^+ eigenspace and converts it to a 2 spinor. This is propagated to time t and then V_t maps the 2 spinor back to the 4-spinor representation. Using the ansatz (10) in the equation of next-to-leading order in \hbar then yields the following transport equation for $b = b_+$:

$$\left[\nabla_p H^+(\nabla_x S^+, \mathbf{x}) \cdot \nabla_x + \frac{\partial}{\partial t} \right] b = -(M_1 + iM_2)b, \quad (11)$$

with the Hermitian 2×2 matrices

$$M_1 := \frac{1}{2} \sum_{j=1}^3 \left(\sum_{k=1}^3 \frac{\partial^2 H^+}{\partial p_j \partial p_k} \frac{\partial^2 S^+}{\partial x_k \partial x_j} + \frac{\partial^2 H^+}{\partial p_j \partial x_j} \right) \mathbb{1}_{2 \times 2},$$

$$M_2 := -\frac{ec}{2\epsilon} \boldsymbol{\sigma} \cdot \mathbf{B} + \frac{ec^2}{2\epsilon(\epsilon + mc^2)} \boldsymbol{\sigma} \cdot (\boldsymbol{\pi} \times \mathbf{E}). \quad (12)$$

We need to solve (11) only along the orbits in phase space, in which case the left-hand side can be viewed as the total time derivative \dot{b} along these orbits. To arrive at (11) we used Coulomb gauge, but this doesn't restrict the result because it only contains the fields \mathbf{E} and \mathbf{B} . The contribution to (11) coming from M_1 is well known from the Schrödinger case [10], and therefore the ansatz

$$b = \sqrt{\det\left(\frac{\partial^2 S^+}{\partial x_j \partial \xi_k}\right)} d, \quad (13)$$

with some 2×2 matrix d , proves useful. From (11) one then obtains the transport equation

$$\dot{d} + iM_2 d = 0, \quad d|_{t=0} = \mathbb{1}_{2 \times 2}, \quad (14)$$

for d , which involves only the spin degrees of freedom.

$$K(\mathbf{x}, \mathbf{y}, t) = \frac{1}{(2\pi i \hbar)^{3/2}} \left[\sum_{\gamma^+_{xy}} V_t d_+ V_0^\dagger D_{\gamma^+_{xy}}^\dagger e^{(i/\hbar)R_{\gamma^+_{xy}}^+ - i(\pi/2)\nu_{\gamma^+_{xy}}} + \sum_{\gamma^-_{xy}} W_t d_- W_0^\dagger D_{\gamma^-_{xy}}^- e^{(i/\hbar)R_{\gamma^-_{xy}}^- - i(\pi/2)\nu_{\gamma^-_{xy}}} \right] \{1 + \mathcal{O}(\hbar)\},$$

$$\text{with } D_{\gamma^\pm_{xy}}^\pm = \sqrt{\left| \det\left(-\frac{\partial^2 R_{\gamma^\pm_{xy}}^\pm}{\partial x_j \partial y_k}\right) \right|}, \quad (15)$$

where γ_{xy}^\pm labels the classical orbits that connect \mathbf{y} and \mathbf{x} in time t . R^\pm is Hamilton's principal function, which is the Legendre transform of S^\pm with respect to $\boldsymbol{\xi}$, and ν^\pm is the Morse index of the corresponding orbit.

We are still left with the calculation of d . Since $d \in \text{SU}(2)$, we can use the representation

$$d = \begin{pmatrix} u & -\bar{v} \\ v & \bar{u} \end{pmatrix} \quad \text{with } |u|^2 + |v|^2 = 1. \quad (16)$$

A candidate for a "classical spin" should be a vector $s \in \mathbb{R}^3$ with fixed length, which we find convenient to choose as $|s| = 1$. We thus seek a map $d \mapsto s$ from $\text{SU}(2)$ to $S^2 \subset \mathbb{R}^3$. To achieve this we propose to use the well known Hopf map $\pi_H: \text{SU}(2) \rightarrow S^2$ defined by

$$\pi_H(d) = s := \begin{pmatrix} 2 \text{Re}(u\bar{v}) \\ 2 \text{Im}(u\bar{v}) \\ |u|^2 - |v|^2 \end{pmatrix} = (\bar{u}, \bar{v}) \boldsymbol{\sigma} \begin{pmatrix} u \\ v \end{pmatrix}. \quad (17)$$

The last equality reveals that s is also connected to a suitable spin expectation value. From (17) and (14) it follows that s fulfills the classical equation

$$\dot{s} = s \times \left[\frac{ec}{\epsilon} \mathbf{B} - \frac{ec^2}{\epsilon(\epsilon + mc^2)} \boldsymbol{\pi} \times \mathbf{E} \right],$$

$$s|_{t=0} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad (18)$$

Because of the unitarity of the time evolution and the initial condition, d has to be an $\text{SU}(2)$ matrix.

The additional phases discussed in [5,6] are caused by M_2 . The second term in M_2 , see (12), can be shown to be $V^\dagger (\nabla_p H^+ \cdot \nabla_x + \frac{\partial}{\partial t}) V$, and thus is a projection of the natural connection on the trivial \mathbb{C}^4 bundle over phase space onto the H^+ eigenbundle. According to [6,12], it hence is the Berry term identified in [5]. We call this $\text{SU}(2)$ Berry term in order to distinguish it from the $\text{U}(1)$ phase originally introduced by Berry [13]. The first term in M_2 then is the "no name term" of [5] that has been shown to be related to a Poisson curvature in [6]. In fact, it measures to what extent the classical time evolution tends to leave the H^+ eigenspace. In physical terms, the first (curvature) term is the interaction of spin and magnetic field, and the second [$\text{SU}(2)$ -Berry] term represents the spin-orbit coupling. Analogous considerations apply to H^- . We remark that we did not need to perform the diagonalization procedure introduced in [5]. Thus the classical orbits are determined by the Hamiltonian (8) and the phases enter separately through (14).

We are now in a position to state the following semiclassical expression for the time evolution kernel:

describing a precessing spin. After [4], this is commonly called Thomas precession; see also [14]. Because of the initial condition, $s \in S^2$ will stay on the northern hemisphere for sufficiently small times. We then choose polar coordinates,

$$s = \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix}, \quad (19)$$

which allows one to calculate d up to a phase η , where $u/|u| = e^{i\eta}$,

$$d = \begin{pmatrix} \cos(\theta/2)e^{i\eta} & -\sin(\theta/2)e^{-i(\eta-\phi)} \\ \sin(\theta/2)e^{i(\eta-\phi)} & \cos(\theta/2)e^{-i\eta} \end{pmatrix}. \quad (20)$$

The equation for η , which is obtained upon inserting (20) into (14) and multiplying by d^\dagger , can immediately be integrated,

$$\eta = \frac{1}{2} \int_0^t s \cdot \left(\frac{ec}{\epsilon} \mathbf{B} - \frac{ec^2}{\epsilon(\epsilon + mc^2)} \boldsymbol{\pi} \times \mathbf{E} \right) dt' + \frac{1}{2} \int_0^t (1 - \cos \theta) \dot{\phi} dt'. \quad (21)$$

The first term is a dynamical phase associated with the energy of a (classical) magnetic moment in given electromagnetic fields, whereas the second term is a geometric

phase. We remark that once s enters the southern hemisphere of S^2 , one should change the phase convention in that $\nu/|\nu| = e^{i\lambda}$ is used to describe the nonclassical degree of freedom. In (21) this amounts to replacing $1/2(1 - \cos\theta)d\phi$ by $-1/2(1 + \cos\theta)d\phi$. These two expressions are the well known gauges of the vector potential for a magnetic monopole of strength $1/2$ situated at the origin of the sphere. The geometric phase caused by this connection is reminiscent of (but not identical to) the quantum mechanical Berry phase of a precessing spin [13].

Now all terms appearing in the semiclassical time evolution kernel are fixed. A nonrelativistic approximation is obtained, if in (15) one keeps only the leading asymptotic term as $c \rightarrow \infty$. As a result, one is left with a block diagonal formula. On the other hand, we also performed the above program of a systematic semiclassical expansion in the case of the Pauli equation. Its result coincides with the upper left block of the former approximation.

Our next goal is to derive a semiclassical trace formula from (15). Since H_D always has a continuous spectrum, which contains at least $(-\infty, -mc^2) \cup (mc^2, \infty)$, we find it convenient to introduce an energy localization such that finally only the discrete spectrum of H_D enters. We thus assume that the spectrum of H_D is purely discrete on an interval $I = (E_a, E_b)$. Then we choose a smooth function $\chi(E)$ which is nonzero only on I , such that $\chi(E_n) = 1$ for all eigenvalues E_n . This can always be achieved if there is no accumulation of eigenvalues at E_a or E_b . Instead of the full time evolution operator we then study its restriction $\chi(H_D)U(t)$. To leading order in \hbar , this restriction only causes additional factors $\chi(E_{\gamma_{xy}})$ in (15). For Schrödinger operators this procedure is described in [10]. The restricted time evolution kernel has a spectral representation

$$\tilde{K}(\mathbf{x}, \mathbf{y}, t) = \sum_n \chi(E_n) \Psi_n(\mathbf{x}) \Psi_n^\dagger(\mathbf{y}) e^{-(i/\hbar)E_n t} \quad (22)$$

with orthonormal eigenspinors Ψ_n . We define a regularized Green's function by

$$\tilde{G}^\ell(\mathbf{x}, \mathbf{y}, E) := \frac{1}{2\pi} \int_{-\infty}^{+\infty} \hat{\varrho}(t) e^{(i/\hbar)Et} \tilde{K}(\mathbf{x}, \mathbf{y}, t) dt, \quad (23)$$

$$\sum_n \chi(E_n) \varrho\left(\frac{E_n - E}{\hbar}\right) = \frac{\hat{\varrho}(0)}{\pi} \frac{|\Omega_E^+| + |\Omega_E^-|}{(2\pi\hbar)^2} \{1 + \mathcal{O}(\hbar)\} + \sum_{\gamma_p^\pm} \frac{\hat{\varrho}(T_{\gamma_p^\pm})}{2\pi} A_{\gamma_p^\pm} e^{(i/\hbar)S_{\gamma_p^\pm}(E) - i(\pi/2)\mu_{\gamma_p^\pm}} \{1 + \mathcal{O}(\hbar)\}$$

with $A_{\gamma_p^\pm} = \frac{2T_{\gamma_p^\pm}^\# \cos(\theta_{\gamma_p^\pm}/2) \cos \eta_{\gamma_p^\pm}}{\sqrt{|\det(M_{\gamma_p^\pm} - \mathbb{1})|}}$. (27)

On the right-hand side the sum extends over the classical periodic orbits γ_p^\pm of energy E . Furthermore, $S(E) = \oint \mathbf{p} \cdot d\mathbf{x}$ is the action, T the period, μ the Maslov index, and M is the (linearized) Poincaré map; $T^\#$ denotes the associated primitive period. We remark that these quantities derive from the relativistic equations of motion

where ϱ is a smooth test function such that its Fourier transform $\hat{\varrho}$ vanishes outside a finite interval. Taking the trace of \tilde{G}^ℓ over spatial variables and matrix components yields

$$\begin{aligned} (\text{Tr } \tilde{G}^\ell)(E) &= \text{Tr}_{4 \times 4} \int_{\mathbb{R}^3} \tilde{G}^\ell(\mathbf{x}, \mathbf{x}, E) d^3x \\ &= \sum_n \chi(E_n) \varrho\left(\frac{E_n - E}{\hbar}\right). \end{aligned} \quad (24)$$

The trace formula can now be derived from (23) and (24) when one introduces the semiclassical approximation (15), but now modified as described above in order to apply to the kernel \tilde{K} . As in the case of the Schrödinger equation, the integrals necessary to calculate (24) can be evaluated with the method of stationary phase. The first and foremost contribution then derives from the stationary points with $t = 0$. In leading semiclassical order this term (also called Weyl term) involves the volumes $|\Omega_E^\pm|$ of the energy shells in phase space,

$$|\Omega_E^\pm| = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \delta[H^\pm(\mathbf{p}, \mathbf{x}) - E] d^3p d^3x. \quad (25)$$

Up to terms $\mathcal{O}(\hbar^\infty)$, all further contributions are caused by the nontrivial periodic orbits of the classical dynamics generated by H^+ and H^- . In the case that all periodic orbits are isolated and unstable (i.e., hyperbolic or inverse hyperbolic) these contributions will be given explicitly. Their calculation is exactly parallel to the case of the Schrödinger equation. The only additional factor that enters comes from the trace over the spin degrees of freedom. If T is the period of a periodic orbit, $V_T = V_0$ so that

$$\begin{aligned} \text{Tr}_{4 \times 4}(V_T d_+ V_0^\dagger) &= \text{Tr}_{2 \times 2}(V_0^\dagger V_T d_+) = \text{Tr}_{2 \times 2} d_+ \\ &= 2 \cos(\theta/2) \cos \eta. \end{aligned} \quad (26)$$

We now choose $E \in I$ such that $\chi(E) = 1$, and thus obtain the trace formula

generated by (8) in the same way as in the nonrelativistic case [9], and thus they are not influenced by the spin. The factor $2 \cos(\theta/2) \cos \eta$ emerging from the spin degrees of freedom has to be interpreted as follows. The angle θ measures the discrepancy between the directions of the spin vector after this has been transported along a given

periodic orbit with the dynamics dictated by (18). The contribution of the periodic orbit to the trace formula is then weighted with $\cos(\theta/2)$. The second term arises from quantum mechanics and, as explained above, is composed of a dynamical as well as of a geometric phase. The factor of 2 finally indicates the presence of two spin directions.

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