Torus quantization for spinning particles

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We derive semiclassical quantization conditions for systems with spin. To this end one has to define the notion of integrability for the corresponding classical system which is given by a combination of the translational motion and classical spin precession. We determine the geometry of the invariant manifolds of this product dynamics which support semiclassical solutions of the wave equation. The semiclassical quantization conditions contain a new term, which is of the same order as the Maslov correction. This term is identified as a rotation angle for a classical spin vector. Applied to the relativistic Kepler problem the procedure shreds some light on the amazing success of Sommerfeld’s theory of fine structure [Ann. Phys. (Leipzig) 51 (1916) 1–94].

PACS numbers: 03.65.Sq, 03.65.Pm, 31.15.Gy

Semiclassical methods for multi-component wave equations have been a topic of constant interest over the last decade, both for their physical applications and the mathematical structures behind them. In a seminal article Littlejohn and Flynn summarized some of the previous efforts in this direction, stressed the importance of geometric or Berry phases in this context and developed a general quantization scheme. Their method, however, does not cover situations in which the so-called principal Weyl symbol of the Hamiltonian has (globally) degenerate eigenvalues. But this problem shows up for the Dirac equation, as we will explain below. It was emphasized by Emmrich and Weinstein that in such a situation integrability of the so-called ray Hamiltonians (which in our case will be given by $H^+$ and $H^-$ defined in eq. (3) below) is not a sufficient condition that allows for an explicit semiclassical quantization. We discuss this problem for the particular case of the Dirac equation, but our method also translates to more general situations.

The semiclassical analysis of the Dirac equation was started by Pauli that in such a situation integrability of the so-called ray Hamiltonians (which in our case will be given by $H^+$ and $H^-$ defined in eq. (3) below) is not a sufficient condition that allows for an explicit semiclassical quantization. We discuss this problem for the particular case of the Dirac equation, but our method also translates to more general situations.

The semiclassical analysis of the Dirac equation was started by Pauli who showed that the rapidly oscillating phase of a WKB-like ansatz has to solve a relativistic Hamilton-Jacobi equation. Later Rubinow and Keller related the amplitude of the semiclassical solution to classical spin precession (i.e. Thomas precession). So far, however, all these efforts did not result in general semiclassical quantization conditions as they were put forward by Keller for the Schrödinger equation. In this article we present the main steps in the derivation of such conditions, finally leading to eq. (10) below. To this end it will be necessary to extend the notion of integrability, see, from Hamiltonian systems to a certain skew product flow which arises naturally in the semiclassical treatment of the Dirac equation. We also illustrate our method for an example, namely the relativistic Kepler problem, which yields Sommerfeld’s fine structure formula.

We first briefly summarize the determination of semiclassical wave functions for the Dirac equation. Details can be found in. Consider the stationary Dirac equation

$$\hat{H}_D = c\alpha \left( \frac{\hbar}{i} \nabla - \frac{e}{c} A(x) \right) + \beta mc^2 + e\phi(x) \quad (1)$$

defined on a suitable domain in $L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$. It describes the motion of a particle with mass $m$, charge $e$ and spin $\frac{1}{2}$ in electro-magnetic potentials $\phi$ and $A$. The Dirac algebra is realized by the $4 \times 4$ matrices

$$\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}, \quad (2)$$

where $\sigma$ is the vector of Pauli matrices and $\mathbb{1}_2$ denotes the $2 \times 2$ unit matrix. We make a semiclassical ansatz of the form

$$\Psi(x) = \left( \sum_{k \geq 0} \left( \frac{\hbar}{i} \right)^k a_k(x) \right) e^{i S(x)} \quad (3)$$

with a scalar phase function $S$ and spinor-valued amplitudes $a_k$. Inserting this ansatz into the Dirac equation and sorting by orders of $\hbar$ in leading order one finds

$$[H_D(\nabla S, x) - E] a_0 = 0 \quad (4)$$

with the matrix-valued function

$$H_D(p, x) = c\alpha \left( p - \frac{e}{c} A(x) \right) + \beta mc^2 + e\phi(x), \quad (5)$$

on classical phase space. The system (4) of linear equations only has a solution with non-trivial $a_0$ if the expression in square brackets has an eigenvalue zero, i.e. if $S$ solves one of the two Hamilton-Jacobi equations $H^\pm(\nabla S, x) = E$ with classical Hamiltonians

$$H^\pm(p, x) = e\phi \pm \sqrt{c^2 \left( p - \frac{e}{c} A \right)^2 + m^2c^4} \quad (6)$$
for particles with positive and negative kinetic energy, respectively. From standard Hamilton-Jacobi theory, see e.g. [4], we conclude that the rapidly oscillating phase of the wave function $[3]$ can be determined by integration along solutions $(P_\pm(t), X_\pm(t))$ of Hamilton’s equations of motion generated by the Hamiltonians $[8]$. Locally we have $P_\pm(t) = \nabla S_\pm(X_\pm(t))$, and thus

$$S_\pm(x) = S_\pm(y) + \int_y^x P_\pm \cdot dx_\pm$$

where we denote by $y = X_\pm(0)$ the (arbitrarily chosen) starting point of integration. If we set $P_0$ to the eigenvalues $H$ of Hamiltonian flows where we denote by $\phi$ for details. For concreteness we now seek a semiclassical solution of (10) can be written as $a_0(x) = V(\nabla S, x)b(x)$ with a $C^2$-valued $b$.

An equation for $b$ can be derived from the next-to-leading order equation, obtained when inserting the semiclassical ansatz $[8]$ into the Dirac equation, by multiplication with $V_\pm$ from the left, cf. $[8]$. (25).

$$(\nabla_p H)\nabla_x b + \frac{i}{2} \sigma B(\nabla_x S, x)b$$

$$+ \frac{ie}{\varepsilon + mc^2} \left( p - \frac{\varepsilon}{c} A \right) \cdot E - \frac{ec}{\varepsilon} B.$$  

(9)

Here we used the abbreviation $\varepsilon := \sqrt{(p - cA)^2 + mc^2}$, and $E(x) = -\nabla \phi(x)$ and $B(x) = \nabla \times A(x)$ denote the electric and magnetic fields, respectively. Viewed as an equation along the orbit $\phi_H^t(\xi, y)$, the first term in (8) constitutes a time derivative along the classical translational dynamics which we shall denote by a dot. The solution of (8) with vanishing $B$ is known to be given by $\sqrt{\det \frac{\partial u}{\partial x}}$, see e.g. [4], and thus the ansatz $b = \sqrt{\det \frac{\partial u}{\partial x}} u$ leaves us with the spin transport equation

$$\dot{u} + \frac{i}{2} \sigma B(\phi_H^t(\xi, y))u = 0.$$  

(10)

The solution of (8) can be written as $u(t) = d(\xi, y, t)u(0)$ with an SU(2)-matrix $d(\xi, y, t)$. We explicitly indicate the dependence on the initial point $(\xi, y)$ of the classical trajectory along which we integrate until time $t$. Through the covering map $\varphi : SU(2) \rightarrow SO(3)$ we can associate with the spin transporter $d$ a rotation matrix $R(\xi, y, t)$, and one easily verifies that $s(t) := R(\xi, y, t)s(0)$ solves the spin precession equation

$$\dot{s} = B(\phi_H^t(\xi, y)) \times s$$  

(11)

on the two-sphere $S^2$ (i.e. $s \in \mathbb{R}^3, |s| = 1$). This is the equation of Thomas precession if we set $\phi_H$ in (8) into the Dirac equation, which defines a flow on the extended classical phase space $\mathbb{R}^{2d} \times S^2$, should be considered as the classical dynamical system corresponding to the Dirac equation, cf. [1].

The key question in semiclassical quantization is now whether it is possible to find a single-valued wave function $\Psi \sim a_0 \exp(iS)$ which solves the above equations. Let us briefly recall the procedure in the sinus pseudocase $[4]$.

In standard semiclassics for the Schrödinger equation one invokes integrability of the classical flow $\phi_H$: Besides the classical Hamiltonian $H =: A_1$ there are $d - 1$ further conserved quantities, $A_2, \ldots, A_d$ (for a system with $d$ degrees of freedom; we only specialize to $d = 3$ later) with mutually vanishing Poisson brackets, $\{A_j, A_k\} = 0$. Then the Theorem of Liouville and Arnold, see [3, chapter 10], guarantees that a (compact and connected) invariant level set $\{ (x, p) | A = \text{const.} \}$ has the topology of a $d$-torus $T^d$ on which the flows $\phi_{A_1}, \ldots, \phi_{A_d}$ generated by $A_1, \ldots, A_d$ commute. By integration along the flow lines of $\phi_{A_1}, \ldots, \phi_{A_d}$ analogous to the integration along $\phi_H$ in (8) – this allows for a definition of the phase function $S$ which is unique up to the contributions of non-contractible loops. Demanding single-valuedness of the semiclassical wave function $\Psi \sim a_0 \exp(iS)$ yields the Einstein-Brillouin-Keller (EBK) quantization conditions

$$\int_{C_j} p \, dx = 2\pi n_j + \frac{\mu_j}{4},$$  

where $\{C_j | j = 1, \ldots, d\}$ denotes a basis of non-contractible loops on the torus characterized by the action variables $I_j = \int_{C_j} p \, dx$. The number $\mu_j \in \{1, 2, 3, 4\}$ is the Maslov index, see [13], of the cycle $C_j$ which, roughly speaking, counts the number of points along $C_j$ at which the pre-factor $\sqrt{\det \frac{\partial u}{\partial x}}$ becomes singular. All these terms also appear in the situation with non-zero spin, and we now have to examine how the spin contribution modifies this picture.

When we include the spin contribution $d(\xi, y, t)$ the situation becomes more complicated and integrability of $\phi_H$ will, in general, not be a sufficient condition to allow for an explicit semiclassical quantization. This can be seen as follows: Transporting the spinor-valued amplitude $u$ along a closed path $C_j$ on a Liouville-Arnold
torus the initial and final value, $u_t$ and $u_f$, respectively, differ not only by a phase but are related by an SU(2)-transformation, $u_t = d_j u_i, d_j \in SU(2)$. Mathematically speaking, we are considering a connection in a $C^2$-bundle with SU(2)-holonomy. If there was only one such loop, as in a system with one translational degree of freedom, we could choose $u_i$ to be an eigenvector of $d_j$, thus reducing the SU(2)-holonomy to a simple phase factor. However, for $d \geq 2$ degrees of freedom this is impossible since the holonomy factors for different loops are, in general, given by non-commuting elements of the holonomy group SU(2). This is a general problem in semiclassics for multi-component wave equations with globally degenerate eigenvalues of the principal symbol, as was emphasized in a general setting by Emmrich and Weinstein [13].

In our situation of semiclassics for spinning particles we will solve this problem by imposing additional conditions on the “field” $B$, which generates the classical spin precession [11]. From a physical point of view it is not surprising that we need a stronger condition than just integrability of the translational dynamics $\phi^t_H$; since we identified the skew product (12) as the classical dynamics corresponding to the Dirac equation, we should also say under which circumstances we want to call the spin dynamics (or rather the combination of translational and spin dynamics) integrable. We do this by the following definition.

**Definition** The skew product $Y^t_{cl}$ is called integrable, if (i) the underlying Hamiltonian flow $\phi^t_H$ is integrable in the sense of Liouville and Arnold and (ii) the flows $\phi^t_{A_1}, \ldots, \phi^t_{A_d}$ can also be extended to skew products $Y^t_{cl,j}$ on $R^{2d} \times S^2$ ($Y^t_{cl} = Y^t_{cl,1}$) with fields $B_j$ fulfilling

$$\{A_j, B_k\} + \{B_j, A_k\} - B_j \times B_k = 0. \quad (14)$$

Condition (14) plays the same role as the condition $\{A_j, A_k\} = 0$ does in the scalar case; it guarantees that all skew products $Y^t_{cl,j}$ commute [14]. Under these conditions we are able to prove the following theorem.

**Theorem** If the skew product flow $Y^t_{cl}$ is integrable, the combined phase space $R^{2d} \times S^2$ can be decomposed into invariant bundles $\mathcal{T}_\theta \rightarrow T^d$ over Liouville-Arnold tori $T^d$ with fiber $S^1$. The bundles can be embedded in $T^{2d} \times S^2$ such that the fibers are characterized by the latitude with respect to a local direction $n(p, x)$, i.e.

$$\mathcal{T}_\theta = \{(p, x, s) \in T^d \times S^2 | \langle s, n(p, x) \rangle = \theta \}. \quad (15)$$

The proof of this theorem will be given elsewhere [13]. The geometry of the the invariant sets $\mathcal{T}_\theta$ is illustrated in figure 1, a Liouville-Arnold torus is sketched as a 2-torus; at two different points we show the attached sphere together with the local axes $n$ and a corresponding parallel of latitude.

If the skew product flow $Y^t_{cl}$ is integrable, the theorem allows us to construct semiclassical wave functions which imply generalized quantization conditions involving the spin degree of freedom. We briefly sketch the construction and then state the quantization conditions. As in the case without spin we define the semiclassical wave function by integration along the flow lines of $\phi^t_{A_1}, \ldots, \phi^t_{A_d}$. In addition we choose the $C^2$-valued part $u$ such that it is an eigenvector of $\sigma n(p, x)$ at each point of the Liouville-Arnold torus $T^d$. (This is only possible if the skew product $Y^t_{cl}$, and not just the Hamiltonian flow $\phi^t_H$, is integrable.) Then the semiclassical wave function is unique up to the contribution of non-contractible loops on $T^d$. Transporting a classical spin vector along such a loop $C_j$ by a combination of the (commuting) skew products $Y^t_{cl,1}, \ldots, Y^t_{cl,d}$, one finds that it is rotated by an angle $\alpha_j$, while integrability of $Y^t_{cl}$ ensures that it stays on the same parallel of latitude. Consequently, the semiclassical wave function is multiplied by a phase factor $e^{\pi i \alpha_j / 2}$, the sign depending on whether we have chosen $u$ to be an eigenvector of $\sigma n$ with eigenvalue $+1$ or $-1$. Demanding single-valuedness of the wave function, the total phase change when moving along a loop $C_j$ has to be an integer multiple of $2\pi$, yielding the quantization conditions

$$\int_{C_j} p \, dx = 2\pi \hbar \left( n_j + \mu j + m_s \frac{\alpha_j}{2\pi} \right), \quad (16)$$

where in addition to the terms in $\{A_1, \ldots, A_d\}$ the spin contribution with the spin quantum number $m_s = \pm \frac{1}{2}$ enters.
We remark that analogous quantization conditions can be derived for the Pauli equation \[14\]. There we can also choose to describe particles with arbitrary spin \( s \in \frac{1}{2}\mathbb{N}_0 \) by replacing the Pauli matrices \( \sigma \) with a higher dimensional irreducible representation of \( \mathfrak{su}(2) \). This changes neither the corresponding classical system (which is always given by a skew product on \( \mathbb{R}^{2d} \times S^2 \)) nor the construction of the semiclassical solutions; only in the quantization conditions \([16]\) the spin quantum number \( m_s \) then takes the values \( -s, -s + 1, \ldots, s \).

We conclude by illustrating these new quantization conditions for a famous example, namely Sommerfeld’s fine structure formula \([13]\). To this end we have to quantize the relativistic Kepler problem with classical Hamiltonian

\[
H(p, x) = -\frac{e^2}{|x|} + \sqrt{c^2p^2 + m^2c^4}.
\]

The problem can be transformed to action and angle variables, see e.g. \([13]\), and the new Hamiltonian depends only on the two action variables \( I_r \) and \( L \). Here \( I_r \) denotes the action variable corresponding to a radial cycle (e.g. from perihelion to aphelion and back), and \( L \) is the modulus of angular momentum \( L = x \times p \).

In 1916 Sommerfeld quantized this system using the old quantum theory, since quantum mechanics was still to be invented, not to think about spin or the Dirac equation. Accordingly, he chose the quantization conditions

\[
I_r = \hbar n_r \quad \text{and} \quad L = \hbar l
\]

with integers \( n_r \in \mathbb{N}_0 \) and \( l \in \mathbb{N} \). More than ten years later it was confirmed that the energy levels resulting from these conditions are exactly the same as one finds by solving the corresponding Dirac equation \([16, 17]\). This is insofar surprising as the Dirac equation not only includes relativistic effects, but also takes into account spin-orbit coupling, which Sommerfeld could not know about. Quantizing the problem with the new conditions \([16]\) yields

\[
I_r = \hbar \left( n_r + \frac{1}{2} \pm \frac{\alpha_r}{2\pi} \right) \quad \text{and} \quad L = \hbar \left( l + \frac{1}{2} \pm \frac{\alpha_L}{2\pi} \right)
\]

with integers \( n_r \) and \( l \) and a Maslov contribution of \( \frac{1}{2} \) for both variables. For the spin rotation angle \( \alpha_r \) we find \( \alpha_L = 2\pi \) for any spherically symmetric system \([13]\). Intriguingly, for the relativistic Kepler problem \( \alpha_r \) is also given by \( 2\pi \)!

Therefore, the conditions \([16]\) and Sommerfeld’s method yield the same values for \( I_r \) and \( L \), thus leading to the same energy levels. A careful analysis of the values that \( n_r \) and \( l \) can assume (one finds \( n_r \geq 0 \) and \( l \geq \frac{1}{2} \pm \frac{1}{2} \)) shows that with the semiclassical quantization scheme developed here one also obtains the correct multiplicities, which Sommerfeld was unable to extract with his method.

Summarizing, we can say that, by a freak of nature, Sommerfeld was able to obtain the correct energy levels of the Dirac hydrogen atom because, roughly speaking, the corrections due to wave mechanics (the Maslov term \( \frac{1}{2} \)) and those due to the spin \( \frac{1}{2} \) of the electron cancel for this particular problem.

I would like to thank Jens Bolte for helpful discussions and I gratefully acknowledge financial support from the Deutsche Forschungsgemeinschaft (DFG) under contract no. Ste 241/10-2.

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