Torus Quantization for Spinning Particles

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We derive semiclassical quantization conditions for particles with spin. These generalize the Einstein-Brillouin-Keller quantization in such a way that, in addition to the Maslov correction, there appears another term which is a remnant of a non-Abelian geometric or Berry phase. This correction is interpreted in terms of a rotation angle for a classical spin vector.

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The WKB (or short-wavelength) approximation is a powerful tool in many branches of physics, which also provides a particularly transparent view on the physical quantities involved. Considering recently renewed interest in spin-related phenomena, e.g., in atomic and condensed matter physics, a semiclassical approach to the Pauli and Dirac equation will potentially prove useful. In this Letter, we present a semiclassical theory for spinning particles which not only yields explicit quantization conditions but also shows that classical equations of motion for a spin vector can provide valuable insight into genuinely quantum mechanical properties.

The semiclassical analysis of the Dirac equation was started by Pauli [1] who showed that the rapidly oscillating phase of a WKB-like ansatz has to solve a relativistic Hamilton-Jacobi equation. Later Rubinow and Keller [2] related the amplitude of the semiclassical solution to classical spin precession (i.e., Thomas precession [3]). 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 [4]. In this Letter, we present the main steps in the derivation of such conditions, finally leading to Eq. (16) below. The crucial point in our approach is to prove the existence of a new constant of motion for integrable systems with spin, namely, the latitude of the classical spin vector with respect to a locally varying direction. We illustrate our method for the relativistic Kepler problem, thus shedding some light on the amazing success of Sommerfeld's theory of fine structure [5].

The problems we are going to discuss have to be viewed in the more general context of semiclassical methods for multicomponent wave equations. These have been a topic of constant interest over the past decade both for their physical applications and the mathematical structures behind them [6–9]. In a seminal article, Littlejohn and Flynn [7] 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 explain below. It was emphasized by Emmrich and Weinstein [8] that in such a situation integrability of the so-called ray Hamiltonians [which in our case are given by H^+ and H^- defined in Eq. (6) below] is not a sufficient condition that allows for an explicit semiclassical quantization. We overcome this problem for the Dirac and Pauli equation by identifying the aforementioned latitude of the classical spin vector as a constant of motion, thus effectively reducing the non-Abelian geometric phase to an ordinary phase factor. The new term in the quantization conditions then depends only on the motion on the fixed parallel of latitude, i.e., on the rotation angle for the classical spin vector.

Let us now first summarize the determination of semiclassical wave functions for the Dirac equation. Details can be found in [2,9,10]. Consider the stationary Dirac equation $\hat{H}_D\Psi = E\Psi$ with Hamiltonian

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

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 electromagnetic potentials ϕ and $\boldsymbol{A}$. The Dirac algebra is realized by the 4×4 matrices

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

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

$$\Psi(\boldsymbol{x}) = \left[\sum_{k\geq 0}\left(\frac{\hbar}{i}\right)^k a_k(\boldsymbol{x})\right] e^{(i/\hbar)S(\boldsymbol{x})} \tag{3}$$

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

$$[H_D(\nabla S, \boldsymbol{x}) - E]a_0 = 0 \tag{4}$$

with the matrix-valued function

$$H_{\mathrm{D}}(\boldsymbol{p},\boldsymbol{x}) = c\boldsymbol{\alpha}\left[\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}(\boldsymbol{x})\right] + \beta mc^2 + e\phi(\boldsymbol{x}), \qquad (5)$$

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

$$H^{\pm}(\boldsymbol{p},\boldsymbol{x}) = e\phi \pm \sqrt{c^2\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 + m^2c^4} \qquad (6)$$

for particles with positive and negative kinetic energy, respectively. From standard Hamilton-Jacobi theory, see, e.g., [11], we conclude that the rapidly oscillating phase of the wave function (3) can be determined by integration along solutions $[\boldsymbol{P}_{\pm}(t), \boldsymbol{X}_{\pm}(t)]$ of Hamilton's equations of motion generated by the Hamiltonians (6). Locally, we have $\boldsymbol{P}_{\pm}(t) = \nabla S^{\pm}[\boldsymbol{X}_{\pm}(t)]$, and thus

$$S^{\pm}(\boldsymbol{x}) = S^{\pm}(\boldsymbol{y}) + \int_{\boldsymbol{y}}^{\boldsymbol{x}} \boldsymbol{P}_{\pm} d\boldsymbol{X}_{\pm}, \qquad (7)$$

where we denote by $\boldsymbol{y} = \boldsymbol{X}_{\pm}(0)$ the (arbitrarily chosen) starting point of integration. If we set $\boldsymbol{\xi} := \boldsymbol{P}_{\pm}(0)$, we can also write $[\boldsymbol{P}_{\pm}(t), \boldsymbol{X}_{\pm}(t)] = \phi^t_{H^{\pm}}(\boldsymbol{\xi}, \boldsymbol{y})$ with the Hamiltonian flows $\phi^t_{H^{\pm}}$. The eigenspaces corresponding to the eigenvalues $H^{\pm}(\boldsymbol{p},\boldsymbol{x})$ of $H_D(\boldsymbol{p},\boldsymbol{x})$ have dimension two and we denote by $V_{\pm}(\boldsymbol{p},\boldsymbol{x})$ the 4×2 matrices of orthonormal eigenvectors, i.e., $V_+^{\dagger}V_+ = \mathbb{1}_2 = V_-^{\dagger}V_-$, $V_+^{\dagger}V_- = 0 = V_-^{\dagger}V_+$, and $V_+V_+^{\dagger} + V_-V_-^{\dagger} = \mathbb{1}_4$; see [10] for details. For concreteness we now seek a semiclassical wave function corresponding to the classical dynamics with H^+ and, in order to simplify notation, drop the index "+". Since Eq. (4) is a matrix equation, it does not only require S to solve the Hamilton-Jacobi equation, but also a_0 to be of the form $a_0(\boldsymbol{x}) = V(\nabla S, \boldsymbol{x})b(\boldsymbol{x})$ with a $\mathbb{C}^2$-valued b.

An equation for b can be derived from the next-to-leading order equation, obtained when inserting the semiclassical ansatz (3) into the Dirac equation, by multiplication with $V_+^{\dagger}$ from the left, cf. [2,9,10],

$$(\nabla_{\boldsymbol{p}}H)\nabla_{\boldsymbol{x}}b + \frac{i}{2}\boldsymbol{\sigma}\boldsymbol{\mathcal{B}}(\nabla_{\boldsymbol{x}}S, \boldsymbol{x})b + \frac{1}{2}\nabla_{\boldsymbol{x}}[\nabla_{\boldsymbol{p}}H(\nabla_{\boldsymbol{x}}S, \boldsymbol{x})]b = 0, \qquad (8)$$

$$\boldsymbol{\mathcal{B}}(\boldsymbol{p},\boldsymbol{x}) := \frac{ec^2}{\varepsilon(\varepsilon + mc^2)}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)\times\boldsymbol{E} - \frac{ec}{\varepsilon}\boldsymbol{B}. \qquad (9)$$

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

$$\dot{u} + \frac{i}{2}\boldsymbol{\sigma}\boldsymbol{\mathcal{B}}[\phi^t_H(\boldsymbol{\xi}, \boldsymbol{y})]u = 0. \qquad (10)$$

The solution of (10) can be written as $u(t) = d(\boldsymbol{\xi}, \boldsymbol{y}, t)u(0)$ with an SU(2)-matrix $d(\boldsymbol{\xi}, \boldsymbol{y}, t)$. We explicitly indicate the dependence on the initial point $(\boldsymbol{\xi}, \boldsymbol{y})$ of the classical trajectory along which we integrate until time t. Through the covering map φ:SU(2) $\rightarrow$ SO(3), we can associate with the spin transporter d a rotation matrix $R(\boldsymbol{\xi}, \boldsymbol{y}, t)$, and one easily verifies that $\boldsymbol{s}(t) := R(\boldsymbol{\xi}, \boldsymbol{y}, t)\boldsymbol{s}(0)$ solves the spin precession equation

$$\dot{\boldsymbol{s}} = \boldsymbol{\mathcal{B}}[\phi^t_H(\boldsymbol{\xi}, \boldsymbol{y})] \times \boldsymbol{s} \qquad (11)$$

on the two-sphere S^2 (i.e., $\boldsymbol{s} \in \mathbb{R}^3$, $|\boldsymbol{s}| = 1$). This is the equation of Thomas precession [3] thus emerging from a semiclassical analysis of the Dirac equation. It turns out that all properties of the semiclassical wave function $\Psi \sim a_0 \exp(\frac{i}{\hbar}S)$ can be determined from the solution $\phi^t_H(\boldsymbol{\xi}, \boldsymbol{y})$ of Hamilton's equations of motion and the solution $\boldsymbol{s}(t)$ of Eq. (11). Thus, the skew product

$$Y^t_{\mathrm{cl}}[\boldsymbol{\xi}, \boldsymbol{y}, \boldsymbol{s}(0)] := [\phi^t_H(\boldsymbol{\xi}, \boldsymbol{y}), R(\boldsymbol{\xi}, \boldsymbol{y}, t)\boldsymbol{s}(0)], \qquad (12)$$

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. [12,13].

The key question in semiclassical quantization is now whether it is possible to find a single-valued wave function $\Psi \sim a_0 \exp(\frac{i}{\hbar}S)$ which solves the above equations. Let us briefly recall the procedure in the spinless case [4].

In standard semiclassics for the Schrödinger equation, one invokes integrability of the classical flow ϕ^t_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 [11], chapter 10, guarantees that a (compact and connected) invariant level set $\{(\boldsymbol{p},\boldsymbol{x}) \mid \boldsymbol{A} = \mathrm{const}\}$ has the topology of a d-torus $\mathbb{T}^d$ on which the flows $\phi^t_{A_1}, \ldots, \phi^t_{A_d}$ generated by $A_1, \ldots, A_d$ commute. By integration along the flow lines of $\phi^t_{A_2}, \ldots, \phi^t_{A_d}$—analogous to the integration along ϕ^t_H in (7)—this allows for a definition of the phase function S which is unique up to the contributions of noncontractible loops. Demanding single-valuedness of the semiclassical wave function $\Psi \sim a_0 e^{(i/\hbar)S}$ yields the Einstein-Brillouin-Keller quantization conditions

$$\oint_{C_j} \boldsymbol{p}d\boldsymbol{x} = 2\pi\hbar\left(n_j + \frac{\mu_j}{4}\right), \qquad n_j \in \mathbb{Z}, \qquad (13)$$

where $\{C_j \mid j = 1, \ldots, d\}$ denotes a basis of noncontractible loops on the torus characterized by the action variables $I_j = \frac{1}{2\pi}\oint_{C_j} \boldsymbol{p}d\boldsymbol{x}$. The number $\mu_j \in \{1, 2, 3, 4\}$ is the Maslov index, see [14], of the cycle C_j which, roughly speaking, counts the number of points along C_j at which the prefactor $\sqrt{\det\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}}$ becomes singular. All these terms also appear in the situation with nonzero spin, and we now have to examine how the spin contribution modifies this picture.

When we include the spin contribution $d(\boldsymbol{\xi}, \boldsymbol{y}, t)$, the situation becomes more complicated and integrability of ϕ_H^t 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_i and u_f, respectively, differ not only by a phase but are related by an SU(2) transformation, $u_f = d_j u_i$, $d_j \in \mathrm{SU}(2)$. Mathematically speaking, we are considering a connection in a $\mathbb{C}^2$ bundle with SU(2) holonomy; i.e., the semiclassical wave function acquires a non-Abelian Berry phase. 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 noncommuting elements of the holonomy group SU(2). This is a general problem in semiclassics for multicomponent wave equations with globally degenerate eigenvalues of the principal symbol, as was emphasized in a general setting by Emmrich and Weinstein [8].

In our situation of semiclassics for spinning particles, we solve this problem by imposing additional conditions on the "field" $\boldsymbol{\mathcal{B}}$, 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 ϕ_H^t; 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_{cl}^t is called integrable, if (i) the underlying Hamiltonian flow ϕ_H^t is integrable in the sense of Liouville and Arnold and (ii) the flows $\phi_{A_2}^t, \ldots, \phi_{A_d}^t$ can also be extended to skew products $Y_{\mathrm{cl}j}^t$ on $\mathbb{R}^{2d} \times S^2$ ($Y_{\mathrm{cl}}^t \equiv Y_{\mathrm{cl}1}^t$) with fields $\boldsymbol{\mathcal{B}}_j$ fulfilling*

$$\{A_j, \boldsymbol{\mathcal{B}}_k\} + \{\boldsymbol{\mathcal{B}}_j, A_k\} - \boldsymbol{\mathcal{B}}_j \times \boldsymbol{\mathcal{B}}_k = 0. \qquad (14)$$

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 $Y_{\mathrm{cl}j}^t$ commute [15]. Under these conditions, we are able to prove the following theorem.

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

$$\mathcal{T}_\theta = \{(\boldsymbol{p}, \boldsymbol{x}, \boldsymbol{s}) \in \mathbb{T}^d \times S^2 \mid \sphericalangle[\boldsymbol{s}, \boldsymbol{n}(\boldsymbol{p}, \boldsymbol{x})] = \theta\}. \qquad (15)$$

The proof of this theorem will be given elsewhere [15]. The geometry of the invariant sets $\mathcal{T}_\theta$ is illustrated in Fig. 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 $\boldsymbol{n}$ and a corresponding parallel of latitude.

If the skew product flow Y_{cl}^t 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 $\phi_{A_1}^t, \ldots, \phi_{A_d}^t$. In addition, we choose the $\mathbb{C}^2$-valued part u such that it is an eigenvector of $\boldsymbol{\sigma n}(\boldsymbol{p}, \boldsymbol{x})$ at each point of the Liouville-Arnold torus $\mathbb{T}^d$. (This is possible only if the skew product Y_{cl}^t, and not just the Hamiltonian flow ϕ_H^t, is integrable.) Then the semiclassical wave function is unique up to the contribution of noncontractible loops on $\mathbb{T}^d$. Transporting a classical spin vector along such a loop C_j by a combination of the (commuting) skew products $Y_{\mathrm{cl}1}^t, \ldots, Y_{\mathrm{cl}d}^t$, one finds that it is rotated by an angle α_j, while integrability of Y_{cl}^t ensures that it stays on the same parallel of latitude. Consequently, the semiclassical wave function is multiplied by a phase factor $e^{\mp i\alpha_j/2}$, the sign depending on whether we have chosen u to be an eigenvector of $\boldsymbol{\sigma n}$ 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 2π, yielding the quantization conditions

$$\oint_{C_j} \boldsymbol{p}\,d\boldsymbol{x} = 2\pi\hbar\left(n_j + \frac{\mu_j}{4} + m_s \frac{\alpha_j}{2\pi}\right), \qquad (16)$$

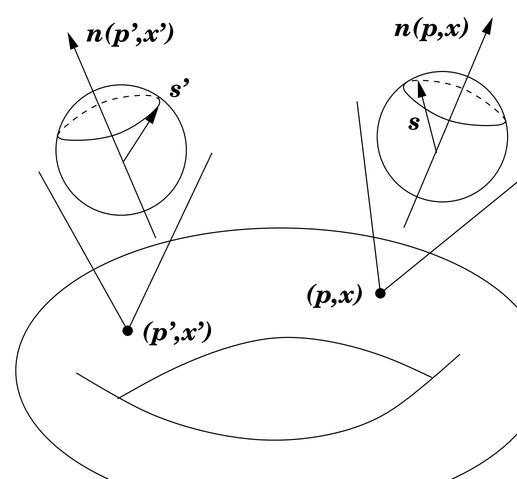

FIG. 1. The invariant manifolds $\mathcal{T}_\theta$ of Y_{cl}^t [see (15)] are given by tori $\mathbb{T}^d$ to which at each point is attached the set of all points on the two-sphere S^2 sharing a fixed latitude θ with respect to a varying axis $\boldsymbol{n}(\boldsymbol{p}, \boldsymbol{x})$.

where, in addition to the terms in (13), 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 [15]. There we can also choose to describe particles with arbitrary spin $s \in \frac{1}{2}\mathbb{N}_0$ by replacing the Pauli matrices $\boldsymbol{\sigma}$ 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 [5]. To this end, we have to quantize the relativistic Kepler problem with classical Hamiltonian

$$H(\boldsymbol{p}, \boldsymbol{x}) = -\frac{e^2}{|\boldsymbol{x}|} + \sqrt{c^2\boldsymbol{p}^2 + m^2c^4}. \qquad (17)$$

The problem can be transformed to action and angle variables, see, e.g., [5], 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 $\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p}$. 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

$$I_r = \hbar n_r \quad \text{and} \quad L = \hbar l, \qquad (18)$$

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

$$I_r = \hbar\left(n_r + \frac{1}{2} \pm \frac{\alpha_r}{4\pi}\right) \quad \text{and} \quad L = \hbar\left(l + \frac{1}{2} \pm \frac{\alpha_L}{4\pi}\right), \qquad (19)$$

with integers n_r and l and a Maslov contribution of $\frac{1}{2}$ for both variables. For the spin rotation angle α_L, we find $\alpha_L = 2\pi$ for any spherically symmetric system [15]. Intriguingly, for the relativistic Kepler problem, α_r is also given by 2π. 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 $l \geq \frac{1}{2} \mp \frac{1}{2}$) 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 have derived semiclassical quantization conditions for particles with both translational and spin degrees of freedom. In order to deal with the non-Abelian Berry phases, which arise in this context, we had to extend the notion of integrability to the combined dynamics of classical translational and spin degrees of freedom. As a consequence, we identified the latitude of the classical spin vector as a constant of motion which allowed us to derive general quantization conditions. Applying the method to the relativistic Kepler problem we found that, by a freak of nature, Sommerfeld obtained 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 that due to the spin of the electron cancel in this particular problem.

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