Experimental Test for Absence of $R$-Term in Schrödinger Equation in Curved Space

H. Kleinert*
Institut für Theoretische Physik,
Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We point out that the presence of a term proportional to the scalar curvature in the Schrödinger equation in curved space can easily be detected in atomic spectra with Russell-Saunders coupling by a violation of the Landé interval rule for adjacent levels $E_J - E_{J-1} \propto J$.

I. INTRODUCTION

In 1957, De Witt presented a derivation of the Schrödinger equation of a point particle in curved space from Feynman’s path integral which contained an extra term proportional to the scalar curvature $R$ in the Hamilton operator:

$$\left( \frac{\hbar^2 \Delta^2}{2M} + c \hbar^2 R \right) \psi(q,t) = i\hbar \partial_t \psi(q,t).$$

As usual, $M$ is the particle mass and $\Delta$ is the Laplace-Beltrami operator. The constant $c$ depends on the way the equation is derived. This was initially nonunique, allowing apparently for different ways of time slicing of the action which led to different values: $c = 1/6, c = 1/12, \ldots, c = 1/8$. The subject is discussed in detail in textbook, where the ambiguity was resolved with the help of a simple novel equivalence principle requiring the absence of the extra $R$ term [i.e. $c = 0$ in (1.1)]. The new principle is deduced from the fact that spaces with curvature (and torsion) can be reached by a nonholonomic, and thus multivalued coordinate transformation, from a flat space. This proceeds by complete analogy with the time-honored Volterra description of defects in crystals and of vortices in superfluids. It is also analogous to Dirac’s generation of string-like magnetic flux tubes by performing multivalued gauge transformation on the electromagnetic vector potential.

There seems to exist a wide-spread belief that it is presently impossible to verify experimentally the absence of an extra $R$-term. This is caused by the fact that one usually thinks of $R$ as the curvature of spacetime in general relativity, which is too small to be detected in a quantum mechanical system, since this extends over a too small spatial region. It is the purpose of this note to point out that there exists a completely different possibility for experimental verification in atomic physics. Atoms whose shell of valence electrons is nearly filled or almost empty, the spins and angular momenta are coupled according to the Russell-Saunders scheme and have an energy described by a Hamilton operator

$$\hat{H} = \frac{1}{2L} \hat{L}^2 + \frac{1}{2S} \hat{S}^2 + \frac{1}{I_{LS}} \hat{L} \cdot \hat{S},$$

where $\hat{L}$ and $\hat{S}$ are the operators of total angular momentum and spin of the electrons, $\hat{L} \cdot \hat{S}$ is the spin-orbit interaction, and $I_L, I_S$ are moments of inertia. The interaction constant $I_{LS}$ is positive for low and negative for high filling.

By calculating the expectation values $\hat{L} \cdot \hat{S}$ in states of total angular momentum $J$ via the commutation rules of the rotation group one finds the eigenvalues

$$2 \hat{L} \cdot \hat{S} = \hat{J}^2 - \hat{L}^2 - \hat{S}^2 = J(J+1) - L(L+1) - S(S+1),$$

which lead to the famous Landé interval rule for adjacent levels $E_J - E_{J-1} = \frac{1}{I_{LS}} J$.}

II. CURVED-SPACE FORMULATION OF HAMILTON OPERATOR

We now show that this well-obeyed rule would be destroyed by an additional $R$-term in the Schrödinger equation with any of the theoretically proposed constants $c \neq 0$. The argument goes as follows. Since Schrödinger quantum

*Email: kleinert@physik.fu-berlin.de, URL: http://www.physik.fu-berlin.de/~kleinert
mechanics is independent of the coordinates used to describe a system, we may consider, for even total spin $S$, the Hamilton operator (1.2) as the quantized version of a classical system in which two point particles of masses $I_L$ and $I_S$ move on a unit sphere. Their Lagrangian has the general form

$$L = \frac{1}{2} \sum_{\mu\nu} g^{\mu\nu} \dot{q}^\mu \dot{q}^\nu,$$  \hspace{1cm} (2.1)$$

where $(q^1, q^2) = (\theta, \varphi)$ and $(q^3, q^4) = (\theta', \varphi')$ are spherical angles, and $g_{\mu\nu}$ is the dynamical metric. The associated Hamiltonian is

$$H = \frac{1}{2} \sum_{\mu\nu} g^{\mu\nu} p_\mu p_\nu,$$  \hspace{1cm} (2.2)$$

where $p_1 = p_\theta = \dot{\theta}$, $p_2 = p_\phi = \sin^2 \theta \dot{\varphi}$ and $p_3 = p_\theta' = \dot{\theta'}$, $p_4 = p_\varphi' = \sin^2 \theta' \dot{\varphi}'$ are the canonical momenta and $g^{\mu\nu}$ is the inverse of the metric $g_{\mu\nu}$.

$$g^{\mu\nu} = \frac{1}{I} \begin{pmatrix} 1 & 0 \\ 0 & \sin^{-2} \theta \end{pmatrix}$$  \hspace{1cm} (2.3)$$

To find the metric associated with the Hamiltonian operator (1.2), we consider for a moment a single point particle of mass $I$ moving on a unit sphere with the Cartesian coordinates $x = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$. Its angular momentum has the components

$$L_1 = -\sin \varphi \dot{\theta} - \sin \theta \cos \varphi \cos \varphi = -\sin \varphi p_\theta - \cot \theta \cos \varphi p_\varphi,$$
$$L_2 = \cos \varphi \dot{\theta} - \sin \theta \cos \varphi \sin \varphi = \cos \varphi p_\theta - \cot \theta \sin \varphi p_\varphi,$$
$$L_3 = \sin^2 \theta \dot{\varphi} = p_\varphi.$$  \hspace{1cm} (2.4)$$

The Hamiltonian can therefore be written as

$$H = \frac{1}{2I} \left( p_\theta^2 + \frac{1}{\sin^2 \theta} p_\varphi^2 \right) = \frac{1}{2} \mathbf{L}^2,$$  \hspace{1cm} (2.5)$$

which has the form (2.2) with the inverse metric

$$g^{\mu\nu} = \frac{1}{I} \begin{pmatrix} 1 & 0 \\ 0 & \sin^{-2} \theta \end{pmatrix}$$  \hspace{1cm} (2.6)$$

By parametrizing the even angular momentum $S$ likewise and forming a combination as in (1.3), we obtain a combined Hamiltonian of the form (2.2) in four dimensions with the following inverse metric

$$g^{\theta\theta} = \frac{1}{I_L}, \quad g_{\theta\phi} = 0, \quad g_{\theta\theta'} = g_{LS} \cos (\varphi - \varphi'), \quad g_{\theta\varphi'} = \frac{2}{I_L} \cot \theta' \sin (\varphi - \varphi'),$$
$$g_{\phi\phi} = \frac{1}{I_L} (1 + \cot^2 \theta), \quad g_{\phi\varphi'} = -\frac{2}{I_L} \cot \theta \sin (\varphi - \varphi'), \quad g_{\phi\varphi'} = \frac{2}{I_L} \cot \theta \cot \theta' \cos (\varphi - \varphi'),$$
$$g_{\varphi\varphi'} = \frac{1}{I_S}, \quad g_{\varphi\varphi'} = 0, \quad g_{\varphi\varphi'} = \frac{1}{I_S} (1 + \cot^2 \theta').$$  \hspace{1cm} (2.7)$$

For this we now calculate the Laplace-Beltrami operator $\Delta = g^{-1/2} (\partial_\mu g^{\mu\nu} g^{1/2} \partial_\nu)$ where $g$ is the determinant of $g_{\mu\nu}$, and find a Schrödinger equation (1.1) in curved space, without an extra $R$-term.
III. EFFECT OF EXTRA R-TERM ON ATOMIC LEVELS

Let us now see how an extra $R$-term would change the spectrum of $\hat{H}$. The calculation of $R$ in this four-dimensional space is quite tedious, but can easily be done with the help of the algebraic computer program Reduce (using the package excalc). The final result is stated most compactly for the limiting case where $I_{LS}^{-1}$ is much smaller than $I_{L}^{-1} + I_{S}^{-1}$. Then we find

$$R = 2\left(\frac{1}{I_{L}} + \frac{1}{I_{S}}\right) + \frac{16}{3} \frac{I_{L} + I_{S}}{I_{LS}} (f - 1),$$

with

$$f = 4 - 6 \sin^{2} \beta,$$

where $\beta$ is the relative angle between $x$ and $x'$. The function $f$ is equal to $\sqrt{5}/16\pi$ times the Clebsch-Gordan combination of the spherical harmonics $Y_{1m}(\theta, \varphi)$ and $Y_{1m'}(\theta', \varphi')$ with a total angular momentum $(J, M) = (2, 0)$. This makes it straight-forward to calculate the matrix elements of $f$ between states of total angular momentum $J$.

The results for $S = 1$ and $L = 1, 2, 3$ are listed in Table I. The table shows that the Landé interval rule would be violated if an extra $R$-term were present in the Schrödinger equation (1.1). We expect that this violation would have been noticed before in the analysis of atomic spectral lines if $c$ had any of the theoretically expected nonzero constants $a$.

Nevertheless it would be interesting to reexamine the validity of the Landé interval rule and derive from this upper bounds for the constant $c$.

Note that in spite of the small factor $\hbar^{2}$ in front of $R$ in the Schrödinger equation (1.1), the shift of levels by (3.1) has the same order of magnitude as the Landé intervals if $c$ and $a, \varepsilon$ are of order unity. This is due to the factors $\hbar^{2}$ in $L^{2}, S^{2}$, and $L \cdot S$.

IV. ACKNOWLEDGMENT

The author thanks Drs. A. Chervyakov and H.J. Schmidt for discussions and Dr. Eberhard Schruefer for helping him to run his Reduce program.

[1] B.S. DeWitt, Rev. Mod. Phys. 29, 337 (1957)
[2] H. Kleinert, Path Integrals in Quantum Mechanics, Statistics and Polymer Physics, World Scientific, Second Edition, Singapore 1995,
[3] H. Kleinert, Gen. Rel. Grav. 32, 769 (2000)
[4] H. Kleinert, Gauge Fields in Condensed Matter, Vol. II, World Scientific, Singapore (1989) (http://www.physik.fu-berlin.de/~kleinert/re0.html#b2)
[5] H. Kleinert, Theory of Fluctuating Nonholonomic Fields and Applications: Statistical Mechanics of Vortices and Defects and Physical Laws in Spaces with Curvature and Torsion, Cambridge Lecture, publ. in Proceedings of NATO Advanced Study Institute on Formation and Interaction of Topological Defects, Plenum Press, New York, 1995, pp. 201–232 (cond-mat/9503030)
[6] See the discussion in the textbook L.D. Landau and E.M. Lifshitz, Quantum Mechanics, Addison-Wesley, New York, 1965, § 72; and R. D. Cowan, The Theory of Atomic Structure and Spectra, University of California Press, Berkeley, 1981.

| $S$ | $L$ | $J$ | $\langle J | f | J \rangle$ | $(E_{J} - E_{J-1})/J$ |
|-----|-----|-----|-----------------|------------------|
| 1   | 1   | 0   | 8/5             | -60/25           |
| 1   | 1   | 1   | -4/5            | 12/25            |
| 1   | 2   | 1   | 4/5             | -28/35           |
| 1   | 2   | 2   | 8/35            | 12/35            |
| 1   | 2   | 3   | 16/25           | -72/150          |
| 1   | 3   | 2   | -4/5            | -20/150          |
| 1   | 3   | 3   | 4/15            |                 |
| 2   | 2   | 0   | 8/7             |                 |
|   |   |   |   |   |
|---|---|---|---|---|
| 2 | 2 | 1 | 4/7 | -84/147 |
| 2 | 2 | 2 | -12/49 | -60/147 |
| 2 | 2 | 3 | -32/49 | -20/147 |
| 2 | 2 | 4 | 16/49 | 36/147 |