Solution of Coulomb Path Integral in Momentum Space

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The path integral for a point particle in a Coulomb potential is solved in momentum space. The solution permits us to give for the first time a negative answer to an old question of quantum mechanics in curved spaces raised in 1957 by DeWitt, whether the Hamiltonian of a particle in a curved space contains an additional term proportional to the curvature scalar \( R \). We show that this would cause experimentally wrong level spacings in the hydrogen atom. Our solution also gives a first experimental confirmation of the correctness of the measure of integration in path integrals in curved space implied by a recently discovered nonholonomic mapping principle.

1. One should think that by now everything interesting is known about the path integral of the Coulomb problem describing the physics of the hydrogen atom. There exists a comprehensive textbook \[1\] in which this subject is treated at great length. However, the existing solution applies only to the fixed-energy amplitude in position space. The momentum space problem has so far remained untackled, and the purpose of this note is to fill this gap.

Apart from our desire to complete the path integral description of the simplest physical object of atomic physics, the present note is motivated by another long-standing open problem in the quantum mechanics of curved spaces, first raised by Bryce DeWitt in 1957 \[2\]: Is the Hamilton operator for a particle in curved space obtained by merely replacing the euclidean Laplace operator in the kinetic energy by the Laplace-Beltrami operator \( \Delta \), or must we add a first raised by Bryce DeWitt in 1957 \[2\]: Is the Hamilton operator for a particle in curved space obtained by merely replacing the euclidean Laplace operator in the kinetic energy by the Laplace-Beltrami operator \( \Delta \), or must we add a

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\[\mathcal{D}f \Phi[f] = f(0).\]

2. Starting point for our treatment is the path integral formulation for the matrix elements in momentum space for the resolvent operator \( \tilde{R} = i/(E - \hat{H}) \) with the Coulomb Hamilton operator \( \hat{H} = \hat{p}^2/2 - \alpha/r \). We use natural units with \( \hbar = M = 1 \), so that masses, lengths, times, and energies will have the units of \( M, \hbar^2/M\alpha, \hbar^3/M\alpha^2 \), and \( M\alpha^2/\hbar^2 \approx 27.21 \text{ eV} \), respectively. The resolvent can be reexpressed as

\[
\tilde{R} = \frac{i}{f(E - H)} \tilde{f}
\]

where \( f \) is an arbitrary function of space, momentum, and some parameter \( s \) \[3\]. Using standard techniques \[3\], the matrix elements of the resolvent are represented by the following canonical euclidean path integral:

\[
(p_{\alpha'}|p_{\alpha})_E = \int_0^\infty dS \int \mathcal{D}^3p \left( \frac{2\pi}{i} \right)^3 \int \mathcal{D}^3x \exp \left\{ -\int_0^S ds \left[ i\dot{\mathbf{p}} \cdot \mathbf{x} + f \left( \frac{\mathbf{p}^2}{2} - E \right) - f\alpha \right] \right\} f(0).
\]

The dot denotes differentiation with respect to \( s \). The left-hand side carries a superscript \( f \) to remind us of the presence of \( f \) on the right-hand side, although the amplitude does not really depend on \( f \). This freedom of choice may be viewed as a gauge invariance \[3\] of (15) under \( f \to f' \). It permits us to subject (15) to an additional path integration over \( f \), as long as a gauge fixing functional \( \Phi[f] \) ensures that only a specific “gauge” contributes. Thus we shall calculate the amplitude as a path integral

\[
(p_{\alpha'}|p_{\alpha})_E = \int \mathcal{D}f \Phi[f] (p_{\alpha'}|p_{\alpha})_E.
\]

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\[ \Phi[f] = \prod_s \frac{1}{r} \exp \left\{ -\frac{1}{2r^2} \left[ f - x^2 \left( \frac{p^2}{2} - E \right) \right]^2 \right\}. \]  

(4)

With this, the total euclidean action in the path integral (3) is

\[ A_{\mathbb{C}}[p, x, \hbar] = \int_0^S \frac{1}{2} ds \left[ i\dot{p} \cdot \dot{x} + \frac{1}{2}x^2 \left( \frac{p^2}{2} - E \right)^2 + \frac{1}{2r^2}f^2 - \frac{1}{r}f \alpha \right]. \]  

(5)

The path integrals over \( f \) and \( x \) in (5) are Gaussian and can be done, in this order, yielding a new euclidean action

\[ A_{\mathbb{C}}[p] = \frac{1}{2} \int_0^S ds \left[ 4p^2 \left( \frac{2\dot{p}^2}{(p^2 + p_E^2)^2} - \alpha^2 \right) \right], \]  

(6)

where we have introduced \( p_E = \sqrt{-2E} \), assuming \( E \) to be negative. The positive regime can always be obtained by analytic continuation. Now, a stereographic projection

\[ \pi \equiv \frac{2pE\dot{p}}{p^2 + p_E^2}, \quad \pi_4 \equiv \frac{p^2 - p_E^2}{p^2 + p_E^2} \]  

transforms (6) to the form

\[ A_{\mathbb{C}}[\pi] = \frac{1}{2} \int_0^S ds \left[ \frac{1}{p_E^2} \pi^2 - \alpha^2 \right], \]  

(8)

where \( \pi \) denotes the four-dimensional unit vectors \((\pi, \pi_4)\). This describes a point particle of pseudomass \( \mu = 1/p_E^2 \) moving on a four-dimensional unit sphere. The pseudotime evolution amplitude of this system is

\[ (\vec{\pi}_b|\vec{\pi}_a) = e^{-Sp_E^2} \int \frac{D^4\pi}{(2\pi)^{3/2}p_E} e^{-A_{\mathbb{C}}[\pi]}. \]  

(9)

There is an exponential prefactor arising from the transformation of the functional measure in (5) to the unit sphere. Let us see how this comes about. When integrating out the spatial fluctuations in going from (5) to (8), the canonical measure in each time slice \( d^3p d^3x/(2\pi)^3 \) becomes \( d^4\pi/(2\pi)^{3/2}(p^2 + p_E^2) \). From the stereographic projection (7) we see that this is equal to \( d^4\pi/(2\pi)^{3/2}p_E^3 \), where \( d^4\pi \) denotes the product of integrals over the solid angle on the surface of the unit sphere in four dimensions, with the integral \( \int d\vec{\pi} \) yielding the total surface \( 2\pi^2 \). From Chapter 10 in the textbook we know that in a curved space, the time sliced measure of path integration is given by the product of invariant integrals \( \int dq\sqrt{|g(q)|} \) in each time slice, multiplied by an effective action contribution \( \exp(-A_{\text{eff}}) = \exp(\int ds R/6\mu) \), where \( R \) is the scalar curvature. For a sphere of radius \( r \) in \( D \) dimensions, \( R = (D-1)(D-2)/r^2 \), implying here \( \exp(-A_{\text{eff}}) = \exp(\int ds 1/\mu) = \exp(\int ds p_E^2) \). Thus, when transforming the time-sliced measure in the original path integral (3) to the time-sliced measure on the sphere in (8) which contains the effective action, the exponent is modified accordingly.

A complete set of orthonormal hyperspherical functions on this sphere may be denoted by \( Y_{nlm}(\vec{\pi}) \), where \( n, l, m \) are the quantum numbers of the hydrogen atom with the well-known ranges \((n = 1, 2, 3, \ldots, \ l = 0, \ldots, n-1, \ m = -l, \ldots, l)\). They can be expressed in terms of the three-dimensional representation \( D^l_{m_1 m_2}(u) \) of the SU(2) matrices \( u = \vec{\pi}\vec{\sigma} \) with the Pauli matrices \( \vec{\sigma} \equiv (1, \sigma^1, \sigma^2, \sigma^3) \) as

\[ Y_{2j+1,l,m}(\vec{\pi}) = \sqrt{\frac{2j+1}{2\pi^2}} \sum_{m_1, m_2 = -j, \ldots, j} (j, m_1; j, m_2) D^{j+1}_{m_1 m_2}(u). \]  

(10)

The orthonormality and completeness relations are

\[ \int d\vec{\pi} Y_{n', l', m'}^*(\vec{\pi}) Y_{n l m}(\vec{\pi}) = \delta_{n n'} \delta_{l l'} \delta_{m m'}, \quad \sum_{n, l, m} Y_{n l m}(\vec{\pi})^* Y_{n l m}(\vec{\pi}) = \delta^{(4)}(\vec{\pi}' - \vec{\pi}). \]  

(11)

where the \( \delta \)-function satisfies \( \int d\vec{\pi} \delta^{(4)}(\vec{\pi}' - \vec{\pi}) = 1 \). When restricting the complete sum to \( l \) and \( m \) only we obtain the four-dimensional analog of the Legendre polynomial:
\[
\sum_{l,m} Y_{nlm}(\vec{\pi}') Y_{nlm}(\vec{\pi}) = \frac{n^2}{2\pi^2} P_n(\cos \vartheta), \quad P_n(\cos \vartheta) = \frac{\sin n\vartheta}{n \sin \vartheta},
\]  

where \( \vartheta \) is the angle between the four-vectors \( \vec{\pi}_b \) and \( \vec{\pi}_a \):

\[
\cos \vartheta = \vec{\pi}_b \cdot \vec{\pi}_a = \frac{(p_b^2 - p_E^2)(p_a^2 - p_E^2) + 4p_b^2 p_d p_a}{(p_b^2 + p_E^2)(p_a^2 + p_E^2)}.
\]  

(13)

The path integral for a particle on the surface of a sphere was solved in [1]. The solution of (9) reads

\[
\langle \vec{\pi}_b | S | \vec{\pi}_a \rangle_0 = (2\pi)^{3/2} \frac{P_E^3}{\pi^2} \sum_{n=1}^{\infty} \frac{n^2}{2\pi^2} P_n(\cos \vartheta) \exp \left\{ -\frac{p_E^2 n^2 + \alpha^2}{2E} \right\}.
\]  

(14)

For the path integral itself in (3), the exponential contains the eigenvalue of the squared angular-momentum operator \( \hat{L}^2/2\mu \) which in \( D \) dimensions is \( l(l + D - 2)/2\mu, \ l = 0, 1, 2, \ldots \). In our system with \( D = 4, l = n - 1 \), these eigenvalues are \( n^2 - 1 \), leading to an exponential \( e^{-p_E^2(n^2 - 1)/2} \). Together with the exponential prefactor in (3), this leads to the exponential in (14). The integral over \( S \) in (13) with (15) can now be done yielding the amplitude at zero fixed pseudoenergy

\[
\langle \vec{\pi}_b | S | \vec{\pi}_a \rangle_0 = -(2\pi)^{3/2} \frac{P_E^3}{\pi^2} \sum_{n=1}^{\infty} \frac{n^2}{2\pi^2} P_n(\cos \vartheta) \frac{2}{2E n^2 + \alpha^2}.
\]  

(15)

This has poles displaying the hydrogen spectrum at energies:

\[
E_n = -\frac{1}{2n^2}, \quad n = 1, 2, 3, \ldots.
\]  

(16)

3. Consider the following generalization of the final action (8):

\[
\mathcal{A}_c[p] = \frac{1}{2} \int_0^S ds \left\{ \frac{1}{h} \frac{4p^2}{(p^2 + p_E^2)^2} - \alpha^2 h \right\}.
\]  

(17)

This action is invariant under reparametrizations \( s \to s' \) if simultaneously \( h \to h ds/ds' \). The path integral with the action (8) in the exponent may thus be rewritten as a path integral with the gauge-invariant action (17) and an additional path integral \( \int dh \Phi[h] \) with an arbitrary gauge-fixing functional \( \Phi[h] \). Going back to a real-pseudo-time parameter \( s = \tau \), the action corresponding to (17) which describes the dynamics of the point particle in the Coulomb potential reads

\[
\mathcal{A}[p] = \frac{1}{2} \int_{\tau_a}^{\tau_b} d\tau \left\{ \frac{1}{h} \frac{4p^2}{(p^2 + p_E^2)^2} + \alpha^2 h \right\}.
\]  

(18)

At the extremum in \( h \), this action reduces to

\[
\mathcal{A}[p] = 2\alpha \int_{\tau_a}^{\tau_b} d\tau \sqrt{\frac{p^2}{(p^2 + p_E^2)^2}}.
\]  

(19)

This is the manifestly reparametrization invariant form of an action in a curved space with a metric \( g^\mu\nu = \delta^\mu\nu / (p^2 + p_E^2)^2 \). In fact, this action coincides with the classical eikonal in momentum space:

\[
S(p_b, p_a; E) = -\int_{p_a}^{p_b} d\tau \dot{p}_x.
\]  

(20)

Observing that the central attractive force makes \( \dot{p} \) point in the direction \(-x\), and inserting \( r = \alpha(p^2 + p_E^2)/2 \), we find precisely the action (18). In fact, the canonical quantization of a system with the action (18) a la Dirac leads directly to a path integral with action (18), [1].
The eikonal, and thus the action, determines the classical orbits via the first extremal principle of theoretical mechanics found in 1744 by Maupertius.

4. Since the Coulomb path integral in momentum space is equivalent to that of a point particle on a sphere, we can use it to pass an experimental judgement on the possible presence of an extra $R$-term in the Hamiltonian operator of the Schrödinger equation in curved space which could be caused by various historic choices of the measure of path integration in the literature. In the exponent of (14), an extra term $c \times \mu \hbar^2 R/2$ in the Hamilton operator in addition to the Laplace-Beltrami term $-\mu \hbar^2 \Delta/2$ would appear as an extra constant $3c$ added to $n^2$. The hydrogen spectrum would then have the energies $E_n = -1/2(n^2 + 3c)$. The only theoretically proposed candidates for $c$ are $1/24$, $1/12$, and $1/8$. The resulting strong distortions of the hydrogen spectrum would certainly have been noticed experimentally a long time ago, apart from the fact that they would contradict Schrödinger theory in $x$-space whose spectrum as the first triumph of quantum theory in atomic physics.

On fundamental level, the present discussion confirms the validity of the nonholonomic mapping principle which predicted the extra factor $\exp(-A_{\text{eff}}) = \exp(\int ds R/6\mu)$ in the measure of the path integral in curved space, without which the correct spectrum in curved momentum space would not have been obtained—the energy would have had the unphysical form $-\alpha/2(n^2 - 1)$ with a singularity at $n = 1$.

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[7] See the discussion in [6] and Chapter 19 of the textbook [1].

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