Group Theory and Orbital Fluctuations of the Hydrogen Atom*

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Abstract

We review some of the progress made made in the past 27 years in understanding the group theoretic and path integral aspects of the hydrogen atom. The group theoretic development was triggered by A.O. Barut who suggested to me the search for a dynamical group larger than $SO(4)$. In this way he became partly responsible also for the later and most recent path integral development.

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1 Introduction

When I met Barut in 1965 in Colorado he suggested to me to try and calculate all dynamical properties of the H atom in terms of group operations within some extension of the symmetry group $SO(4)$. In this way I should be able to avoid the use of the full algebra of canonical position and momentum operators $\hat{x}, \hat{p}$. The first idea was to relate the matrix elements of $\hat{p}$ and $\hat{x}$ to those of generators of a Lie algebra extending that of $SO(4)$. However, when evaluating the matrix elements of the position operator on the H atom wave function there was an immediate obstacle: The operator $\hat{x}$ connected all principal quantum numbers n with each other. Generators of a Lie algebra, on the other hand, always transform states into those with neighboring quantum numbers. This is a fundamental consequence of the binary structure of the commutation relations. Thus a finite group operation had to intervene to achieve the goal. This transformation was soon found. The H wave functions are proportional to those of the harmonic oscillator, except for a factor $1/n$ in the argument. I therefore removed this factor by a scale transformation. After this the matrix elements of $\hat{x}, \hat{p}$ did indeed connect only neighboring n. They turned out to be generators of the Lie algebra of the group $SO(4,2)$. There are 15 generators denoted by L_{AB} with $L_{AB} = -L_{BA}$ and $A, B = 1, \ldots, 6$. The scale transformation turned out to be a finite element within this group, the *tilt operator* $\hat{T} \equiv e^{iL_{56} \log n}$. The existence of this operator was essential for accommodating the continuous states of the H atom in the oscillator Hilbert space. The oscillator wave functions $\psi_n(\mathbf{x})$ are complete. The rescaled ones $\psi_n(\mathbf{x}/n)$, however, which describe the bound states of the H atom are not. The loss of completeness is due to the following fact: While for large n, the oscillator wave functions $\psi_n(\mathbf{x})$ oscillate more and more rapidly and are capable of building up a local wave packet, this is no longer true for the rescaled wave functions $\psi_n(\mathbf{x}/n)$. In these, the higher n waves are "pulled apart" proportionally to n and this prevents them from acquiring large enough wave numbers to build up a local packet. The gap in the Hilbert space arising from this rescaling is filled precisely by the continuum wave functions. These insights were obtained in 1965 and comprehensive reviews were published in 1968 [1].

The so gained understanding of the oscillator properties of the H atom wave functions was essential to the more recent development of a path integral approach to the H atom. As I explained in the preface of my textbook on path integrals [2], I was approached by Feynman in 1972 who suggested looking at the problem during my sabbatical at Caltech in 1972. I did not follow this suggestion until 1978 when I had to teach a course on quantum mechanics at my home university in Berlin. At that time it had become customary to present in such a course at least a brief introduction into path integrals and to explain the concept of quantum fluctuations. At the same time, I.H. Duru had joined my group as a postdoc from Turkey on a Humboldt fellowship. He had learned the quantum mechanics of the H atom in a previous collaboration with Barut. I therefore suggested to him the collaboration on the path integral. He quickly acquired the basic techniques and very soon we found the most important ingredient of the solution [3]: The transformation of time in the path integral to a new path dependent pseudotime, combined with a transformation of the coordinates to "square-root coordinates" via a Kustaanheimo-Stiefel transformation. Unfortunately, we were able to perform these transformations only in a very formal way which led to the correct result, as we now know, only due to good fortune. Our procedure was soon criticized [4] because of the sloppy treatment of the time slicing. A proper treatment could, in principle, have rendered unwanted corrections which we had simply ignored. Some authors went through a detailed time-slicing procedure [5] but the correct result emerged only by transforming the measure of path integration inconsistently. In fact, when I calculated the corrections according to the standard rules I found them to be zero only in $D = 2$ dimensions [6]. The same treatment in $D = 3$ dimensions gave non-zero corrections which spoiled the beautiful result and left me puzzled. Only very recently I happened to locate the place where the $D = 3$ treatment failed: It was the transformation of the time-sliced measure in the path integral from the original cartesian to the auxiliary "square-root coordinates" in which the system becomes harmonic and integrable. In contrast to $D = 2$, the $D = 3$ transformation is non-holonomic and introduces not only curvature but also torsion. This suggested that the transformations of the time-sliced measure had a hitherto unknown dependence on torsion. Thus it was essential to find first the correct path integral for a particle moving in a space with curvature and torsion. This was a non-trivial task since already in a space with curvature only, the literature was ambiguous giving several prescriptions to choose from which differed by multiples of the curvature scalar added to the energy [7]. The ambiguities are path integral analogs of the so-called operator ordering problem in quantum mechanics. When trying to apply any of the existing prescriptions to spaces with torsion, I always ran into disaster finding non-covariant answers. So, something had to be wrong with all of them. Guided by the idea that in spaces with constant curvature the path integral should give the same result as the operator quantum mechanics based on the commutation rules of the generators of angular momentum I was eventually able to find a consistent *quantum equivalence principle* for path integrals [8], thus giving a unique answer also to the operator ordering problem. This finally enabled me to solve the leftover problem of the $D = 3$ H atom path integral, the absence of the finite time-slicing corrections.

Let us review some aspects of this development.

2 Schrödinger Theory

The Schrödinger equation of the H atom is

$$\left(-\frac{1}{2M}\hbar^2\partial_{\mathbf{x}}{}^2 - E\right)\psi(\mathbf{x}) = \frac{e^2}{r}\psi(\mathbf{x}). \tag{1}$$

Multiplying this by a regulating function $f = r$ from the left gives

$$\left(-\frac{1}{2M}\hbar^2 r\partial_{\mathbf{x}}{}^2 - Er\right)\psi(\mathbf{x}) = e^2\psi(\mathbf{x}). \tag{2}$$

This equation can be transformed into the Schrödinger equation of the four-dimensional harmonic oscillator as follows. First one introduces a dummy forth coordinate x^4, extends the Hilbert space accordingly, and compensates for this by restricting the physical wave functions to be independent of x^4. This implies the constraint:

$$\partial_{x^4}\psi = 0. \tag{3}$$

Then one extends the derivative term in (2) to

$$\partial_{\mathbf{x}}^2 + \partial_{x^4}^2 \equiv \partial_i^2, \qquad i = 1,2,3,4. \tag{4}$$

After this one goes over to the square-root coordinates u^μ via a *Kustaanheimo-Stiefel transformation* which has been used for a long time in celestial mechanics. Every point $\mathbf{x}$ in space is mapped into a 4-dimensional u^μ-space ($\mu = 1,2,3,4$) via the following equations

$$x^i = \bar{z}\sigma^i z, \qquad r = \bar{z}z. \tag{5}$$

Here

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{6}$$

are the Pauli matrices and $z, \bar{z}$ the two-component objects

$$z = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}, \quad \bar{z} = (z_1^*, z_2^*), \tag{7}$$

called "spinors". Their components are related to the four-vector u^μ by

$$z_1 = (u^1 + iu^2), \quad z_2 = (u^3 + iu^4) \tag{8}$$

The coordinates u^μ can be parametrized in terms of the spherical angles of the three-vector $\mathbf{x}$ plus one additional arbitrary angle γ as follows

$$\begin{aligned} z_1 &= \sqrt{r}\cos(\theta/2)e^{-i[(\varphi+\gamma)/2]}, \\ z_2 &= \sqrt{r}\sin(\theta/2)e^{i[(\varphi-\gamma)/2]}. \end{aligned} \tag{9}$$

In the equations (5), the angle γ obviously cancels. This is why each point in x^i-space corresponds to an entire curve in u^μ-space, with $\gamma \in [0, 4\pi]$. We can write (5) also in the matrix form

$$\begin{pmatrix} x^1 \\ x^2 \\ x^3 \end{pmatrix} = A(\vec{u}) \begin{pmatrix} u^1 \\ u^2 \\ u^3 \\ u^4 \end{pmatrix}, \tag{10}$$

with the 3×4 matrix

$$A(\vec{u}) = \begin{pmatrix} u^3 & u^4 & u^1 & u^2 \\ u^4 & -u^3 & -u^2 & u^1 \\ u^1 & u^2 & -u^3 & -u^4 \end{pmatrix}. \tag{11}$$

Since

$$r = (u^1)^2 + (u^2)^3 + (u^3)^2 + (u^4)^2 \equiv (\vec{u})^2, \tag{12}$$

this transformation certainly makes the potential $-Er$ in (2) harmonic in $\vec{u}$. We have indicated the four-vector nature of u^μ by a vector-symbol on top, $\vec{u}$.

Consider now the derivative term in (2). The mapping of the tangent vectors du^μ into dx^i is given by

$$\begin{pmatrix} dx^1 \\ dx^2 \\ dx^3 \end{pmatrix} = 2 \begin{pmatrix} u^3 & u^4 & u^1 & u^2 \\ u^4 & -u^3 & -u^2 & u^1 \\ u^1 & u^2 & -u^3 & -u^4 \end{pmatrix} \begin{pmatrix} du^1 \\ du^2 \\ du^3 \\ du^4 \end{pmatrix}. \tag{13}$$

A classical kinetic term requires solving this equation for dx^i. This is possible only after specifying the differential of the dummy angle $d\gamma$. To do so we find it convenient to replace $d\gamma$ by a parameter which is more naturally related to the dx^i's on the left-hand side. We embed the tangent vector (dx^1, dx^2, dx^3) into a fictitious four-dimensional space and define the new fourth component dx^4 by an additional forth row in the matrix $A(\vec{u})$, extending it to a 4×4 equation

$$d\vec{x} = 2A(\vec{u})d\vec{u} \tag{14}$$

The vector symbol on top of x indicates that it is now also a four-vector x^i. For symmetry reasons, we choose the 4×4 matrix $A(\vec{u})$ to be as follows

$$A(\vec{u}) = \begin{pmatrix} u^3 & u^4 & u^1 & u^2 \\ u^4 & -u^3 & -u^2 & u^1 \\ u^1 & u^2 & -u^3 & -u^4 \\ u^2 & -u^1 & u^4 & -u^3 \end{pmatrix}. \tag{15}$$

The forth row implies the following relation between dx^4 and $d\gamma$

$$\begin{aligned} dx^4 &= 2(u^2du^1 - u^1du^2 + u^4du^3 - u^3du^4) \\ &= r(\cos\theta\ d\varphi + d\gamma). \end{aligned} \tag{16}$$

We write the transformations (14) as $dx^i = e^i{}_\mu(\mathbf{u})\, du^\mu$ with now $i = 1, 2, 3, 4$, with the basis tetrad

$$e^i{}_\mu(\mathbf{u}) = \frac{\partial x^i}{\partial u^\mu} = 2A^i{}_\mu(\mathbf{u}), \tag{17}$$

define a metric in u^μ space by

$$g_{\mu\nu} \equiv e^i_\mu e^i_\nu \tag{18}$$

and the reciprocal tetrad by

$$e^i{}_\mu(\mathbf{u}) e_i{}^\nu = \delta_\mu{}^\nu. \tag{19}$$

From these we calculate the connection in the u^μ-space

$$\Gamma_{\mu\nu}{}^\lambda = e_i{}^\lambda \partial_\mu e^i{}_\nu \tag{20}$$

which will play an important role later.

Observe that the relation (16) is not integrable since $\partial x^4/\partial u^1 = 2u^2$, $\partial x^4/\partial u^2 = -2u^1$, and hence

$$(\partial_{u^1}\partial_{u^2} - \partial_{u^2}\partial_{u^1})x^4 = -4,$$

with similar relations for other pairs of components. It is a non-holonomic mapping which changes the euclidean geometry of the four-dimensional $\vec{x}$-space into a non-euclidean $\vec{u}$-space with curvature and torsion. This will be discussed in detail in Sec ??. Here we only note that the impossibility of finding a unique mapping between the *points* of $\vec{x}-$ and $\vec{u}$-space reflects itself in a mapping between *paths* only in a multivaluedness of the initial points. After a choice has been made for those, the mapping (14) specifies the image path uniquely. Under the Kustaanheimo-Stiefel transformation, the extended gradient term (4) in the Eq. (2) goes over into $g^{\mu\nu}\partial_\mu\partial_\nu - \Gamma_\mu{}^{\mu\lambda}\partial_\lambda$. With the property $\Gamma_\mu{}^{\mu\lambda} = 0$, the second term is absent and the result is simply $g^{\mu\nu}\partial_\mu\partial_\nu$. Since $g^{\mu\nu} = \delta^{\mu\nu}/4r$ the Schrödinger equation (2) goes directly over into

$$\left[-\frac{1}{8M}\hbar^2\partial_\mu^2 - E(u^\mu)^2\right]\psi(u^\mu) = e^2\psi(u^\mu). \tag{21}$$

With $\mu = 4M$ and $-E = \mu\omega^2/2$ this is the Schrödinger equation of an harmonic oscillator

$$\left[-\frac{1}{2\mu}\hbar^2\partial_\mu^2 + \frac{\mu}{2}\omega^2(u^\mu)^2\right]\psi(u^\mu) = \mathcal{E}\psi(u^\mu). \tag{22}$$

The eigenvalues of the pseudoenergy $\mathcal{E}$ are

$$\mathcal{E}_N = \hbar\omega(N + D_u/2), \tag{23}$$

where D_u is the dimension of u^μ-space and

$$N = \sum_{i=1}^{D_u} n_i \tag{24}$$

is the sum of the integer quantum numbers for each direction of u^μ-space. Because of the multivaluedness of the mapping from $\mathbf{x}$ to u^μ, only symmetric wave functions can be associated with H atom states, Hence N must be even and can be written as $N = 2(n-1)$ with $n = 1, 2, 3, \ldots$. The pseudoenergy spectrum is therefore

$$\mathcal{E}_n = \hbar\omega 2(n + D_u/4 - 1), \quad n = 1, 2, 3, \ldots \ . \tag{25}$$

According to (22) the H atom wave functions must all have a pseudoenergy

$$\mathcal{E}_n = e^2. \tag{26}$$

The two equations are fulfilled if the oscillator frequency has the discrete values

$$\omega = \omega_n \equiv \frac{e^2}{2(n + D_u/4 - 1)}, \quad n = 1, 2, 3 \ldots \ . \tag{27}$$

With $\omega^2 = -E/2M$ this implies the H atom energies

$$E_n = -2M\omega_n^2 = -\frac{Me^4}{\hbar^2}\frac{1}{2(n + D_u/4 - 1)^2}. \tag{28}$$

showing that the number $n = N/2$ plays the role of the principal quantum number of the H atom wave functions.

Let us now focus our attention only on the three-dimensional H atom with $D_u = 4$. In this case not all even oscillator wave functions correspond to H atom bound-state wave functions. This follows from the fact that the H atom wave functions do not depend on the dummy forth coordinate x^4 (or the dummy angle γ). Thus they satisfy the constraint $\partial_{x^4}\psi = 0$, implying in u^μ-space [recall (185)],

$$\begin{aligned} -ir\partial_{x^4}\psi(\mathbf{x}) &= -ire_4{}^\mu\partial_\mu\psi(u^\mu) \equiv \\ \hat{L}_{05}\psi(u^\mu) &= -i\frac{1}{2}\left[(u^2\partial_1 - u^1\partial_2) + (u^4\partial_3 - u^3\partial_4)\right]\psi(u^\mu) \\ &= -i\partial_\gamma\psi(u^\mu) = 0. \end{aligned} \tag{29}$$

The explicit construction of the oscillator and H atom bound-state wave functions is most conveniently done in terms of the complex coordinates (8). Then the constraint (29) becomes

$$\hat{L}_{05}\psi(z,z^*) = \frac{1}{2}\left[\bar{z}\partial_{\bar{z}} - z\partial_z\right]\psi(z,z^*) = 0, \tag{30}$$

which will be used below to select the H atom states.
To simplify the notation we go over to atomic units with $\hbar = 1, M = 1, e^2 = 1$ in which $\mu = 4M = 4$, lengths are measured in units of the Bohr radius $a_H = \hbar^2/Me^2$, energies in units of Rydberg $Ry \equiv E_H = e^2/a_H = Me^4/\hbar^2$, and ω in units of $\omega_H \equiv e^2/\hbar\sqrt{2}$. Then the Schrödinger equation (21) reads (after multiplication by $4M/\hbar^2$),

$$\hat{h}\psi(u^\mu) \equiv \frac{1}{2}\left[-\partial_\mu^2 + 16\omega^2(u^\mu)^2\right]\psi(u^\mu) = 4\psi(u^\mu). \tag{31}$$

The spectrum of the operator $\hat{h}$ is $4\omega(N+2) = 8\omega n$ so that the H atom bound states satisfy $\omega = \omega_n = 1/2n$ (in unit ω_H).

We now observe that the operator $\hat{h}$ can be brought to the following standard form

$$\hat{h}^s = \frac{1}{2}\left[-\partial_\mu^2 + 4(u^\mu)^2\right], \tag{32}$$

by an ω dependent transformation

$$\hat{h} = 4\omega e^{i\vartheta\hat{D}}\hat{h}^s e^{-i\vartheta\hat{D}}, \tag{33}$$

where the operator $\hat{D}$ is the infinitesimal dilatation operator, also called *tilt operator* [1]

$$\hat{D} \equiv -\frac{1}{2}iu^\mu\partial_\mu, \tag{34}$$

and ϑ is the *tilt angle*,

$$\vartheta = \log(2\omega). \tag{35}$$

The wave functions are therefore given by the rescaled solutions of the standardized Schrödinger equation (32),

$$\psi(u^\mu) = e^{i\vartheta\hat{D}}\psi^s(u^\mu) = \psi^s(\sqrt{2\omega}u^\mu). \tag{36}$$

Notice that the rescaling depends on ω and thus on the principal quantum number n, so that

$$\psi_n(u^\mu) = \psi_n^s(u^\mu/\sqrt{n}). \tag{37}$$

The standardized wave functions $\psi_n^s(u^\mu)$ are constructed most conveniently by means of four sets of creation and annihilation operators $\hat{a}_1^\dagger, \hat{a}_2^\dagger, \hat{b}_1^\dagger, \hat{b}_2^\dagger$, $\hat{a}_1, \hat{a}_2, \hat{b}_1, \hat{b}_2$. They are made up of z_1, z_2, their complex conjugates, and the associated differential operators. In addition, we choose the indices so that a_i and b_i transform in the same way under the the spinor representation of the rotation group. If c_{ij} is the 2×2 matrix

$$c = i\sigma^2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{38}$$

then $c_{ij}z_j$ transforms like z_i^*. We therefore define the creation operators

$$\begin{aligned} \hat{a}_1^\dagger &= -\frac{1}{\sqrt{2}}(-\partial_{z_2^*} + z_2), \qquad \hat{b}_1^\dagger = \frac{1}{\sqrt{2}}(-\partial_{z_1} + z_1^*), \\ \hat{a}_2^\dagger &= \frac{1}{\sqrt{2}}(-\partial_{z_1^*} + z_1), \qquad \hat{b}_2^\dagger = \frac{1}{\sqrt{2}}(-\partial_{z_2} + z_2^*), \end{aligned} \tag{39}$$

and the annihilation operators (note that $\partial_z^\dagger = -\partial_{z^*}$)

$$\begin{aligned} \hat{a}_1 &= -\frac{1}{\sqrt{2}}(\partial_{z_2} + z_2^*), \qquad \hat{b}_1 = \frac{1}{\sqrt{2}}(\partial_{z_1^*} + z_1), \\ \hat{a}_2 &= \frac{1}{\sqrt{2}}(\partial_{z_1} + z_1^*), \qquad \hat{b}_2 = \frac{1}{\sqrt{2}}(\partial_{z_2^*} + z_2). \end{aligned} \tag{40}$$

The standardized oscillator Hamiltonian is then

$$\hat{h}^s = \hat{a}^\dagger \hat{a} + \hat{b}^\dagger \hat{b} + 1, \tag{41}$$

where we have used spinor notation, as in (5). The ground state of the four-dimensional oscillator is annihilated by $\hat{a}_1, \hat{a}_2; \hat{b}_1, \hat{b}_2$, and has therefore the wave function

$$\langle z, z^* | 0 \rangle = \psi_{s,0000}(z, z^*) = \frac{1}{\sqrt{\pi}} e^{-z_1 z_1^* - z_2 z_2^*} = \frac{1}{\sqrt{\pi}} e^{-(u^\mu)^2}. \tag{42}$$

The complete set of oscillator wave functions is obtained, as usual, by applying the creation operators to the ground state,

$$|n_1^a, n_2^a, n_1^b, n_2^b\rangle = N_{n_1^a,n_2^a,n_1^b,n_2^b}\; \hat{a}_1^{\dagger n_1^a} \hat{a}_2^{\dagger n_2^a} \hat{b}_1^{\dagger n_1^b} \hat{b}_2^{\dagger n_2^b} |0\rangle, \tag{43}$$

with

$$N_{n_1^a,n_2^a,n_1^b,n_2^b} = \frac{1}{\sqrt{n_1^a! n_2^a! n_1^b! n_2^b!}}. \tag{44}$$

The principal quantum number n is given by the sum of all quanta

$$n = n_1^a + n_2^a + n_1^b + n_2^b + 1. \tag{45}$$

The H atom bound-state wave functions arise only from those oscillator wave functions which satisfy the constraint (30). This reads now

$$\hat{L}_{05} = -\frac{1}{2}(\hat{a}^\dagger \hat{a} - \hat{b}^\dagger \hat{b})\psi^s = 0. \tag{46}$$

Thus the H atom states carry an equal number of a and b quanta. They diagonalize the (mutually commuting) a and b spins

$$\hat{L}_i^a \equiv \frac{1}{2}\hat{a}^\dagger \sigma_i \hat{a}, \quad \hat{L}_i^a \equiv \frac{1}{2}\hat{b}^\dagger \sigma_i \hat{b}, \tag{47}$$

with the quantum numbers

$$\begin{aligned} l^a &= (n_1^a + n_2^a)/2, \quad & m^a &= (n_1^a - n_2^a)/2, \\ l^b &= (n_1^b + n_2^b)/2, \quad & m^b &= (n_1^b - n_2^b)/2, \end{aligned} \tag{48}$$

where l, m are, as usual, the eigenvalues of $\hat{L}^2$ and $\hat{L}_3$. This gives the correct degeneracy n^2 for the states with principal quantum number n. By defining

$$\begin{aligned} &n_1^a \equiv n_1 + m, \quad n_2^a \equiv n_2, \quad n_1^b = n_2 + m, \quad n_2^b = n_1, \qquad \text{for } m \geq 0, \\ &n_1^a \equiv n_1, \quad n_2^a \equiv n_2 - m, \quad n_1^b = n_2, \quad n_2^b = n_1 - m, \qquad \text{for } m \leq 0, \end{aligned} \tag{49}$$

we establish contact with the wave functions which arise naturally when diagonalizing the H atom Hamiltonian in parabolic coordinates. The relation between these states and the usual H atom wave function of given angular momentum $|nlm\rangle$ is obvious by observing that the angular momentum operator $\hat{L}_i$ is equal to the sum of a and b spins. The rediagonalization is therefore achieved by the usual vector coupling coefficients.

Notice that after the tilt transformation (36), exponential behavior of the oscillator wave functions $\psi_n^s(u^\mu) \propto \text{polynomial}(u^\mu u^\nu) \times e^{-(u^\mu)^2}$ go correctly over into the well-known behavior of the H atom wave functions $\psi(\mathbf{x}) \propto \text{polynomial}(\mathbf{x}) \times e^{-r/n}$.

It is important to realize that although the dilation operator $\hat{D}$ is hermitian and the operator $e^{i\vartheta\hat{D}}$ unitary for *fixed* ϑ, the H atom bound states ψ_n, which arise from the complete set of oscillator states ψ_n^s by an n-dependent tilt angle $\vartheta_n = \log(1/n)$, do *not* span the Hilbert space. A piece of the space is left out. The continnum states of the H atom precisely fill the gap. Intuitively we can understand this as follows: The oscillator wave functions $\psi_n^s(u^\mu)$ oscillate in space with shorter and shorter wavelength for increasing n. This is why the completeness sum $\sum_n \psi_n^s(u^\mu)\psi_n^{s*}(u^\mu)$ can build up a δ-function necessary to span the space. In the sum of the dilated wave functions, however,

$$\sum_n \psi_n^s(u^\mu/\sqrt{n})\psi_n^{s*}(u^\mu/\sqrt{n}),$$

the terms of larger n have increasingly stretched spatial oscillations and these no longer suffice to build up an infinitely narrow distribution.

3 Group Theory

The subspace of oscillator states in the standardized form (36), $\psi^s(u^\mu/\sqrt{n})$, which do not depend on x^4 (i.e., on γ) are obtained by applying an equal number of creation operators $a^\dagger$ and $b^\dagger$ to the ground state as in Eq. (43). These states form an irreducible representation of the dynamical group $O(4,2)$. The 15 generators $\hat{L}_{AB} \equiv -\hat{L}_{BA}$, $A, B = 1, \ldots 6$ of this group are constructed from the spinors

$$\hat{a} \equiv \begin{pmatrix} \hat{a}_1 \\ \hat{a}_2 \end{pmatrix}, \quad \hat{b} \equiv \begin{pmatrix} \hat{b}_1 \\ \hat{b}_2 \end{pmatrix}, \tag{50}$$

and their hermitian adjoints using the Pauli σ-matrices and $c \equiv i\sigma^2$ as follows ($\sigma_i \equiv \sigma^i$):

$$\hat{L}_{ij} = \frac{1}{2}\left(\hat{a}^\dagger\sigma_k\hat{a} + \hat{b}^\dagger\sigma_k\hat{b}\right) \quad i, j, k = 1, 2, 3 \text{ cyclic},$$

$$
\begin{aligned}
\hat{L}_{i4} &= \frac{1}{2}\left(\hat{a}^\dagger \sigma_i \hat{a} - \hat{b}^\dagger \sigma_i \hat{b}\right), \\
\hat{L}_{i5} &= \frac{1}{2}\left(\hat{a}^\dagger \sigma_i c \hat{b}^\dagger - \hat{a} c \sigma_i \hat{b}\right), \\
\hat{L}_{i6} &= \frac{i}{2}\left(\hat{a}^\dagger \sigma_i c \hat{b}^\dagger + \hat{a} c \sigma_i \hat{b}\right), \\
\hat{L}_{45} &= \frac{1}{2i}\left(\hat{a}^\dagger c \hat{b}^\dagger - \hat{a} c \hat{b}\right), \\
\hat{L}_{46} &= \frac{1}{2}\left(\hat{a}^\dagger c \hat{b}^\dagger + \hat{a} c \hat{b}\right), \\
\hat{L}_{56} &= \frac{1}{2}\left(\hat{a}^\dagger \hat{a} + \hat{b}^\dagger \hat{b} + 2\right).
\end{aligned} \tag{51}
$$

The commutation rules of these operators are

$$
[\hat{L}_{AB}, \hat{L}_{AC}] = i g_{AA} \hat{L}_{BC}, \tag{52}
$$

where

$$
g_{AB} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} \tag{53}
$$

is the metric of the $O(4,2)$ defining representation. It can be verified that the following combinations of position and momentum operators are elements of the Lie algebra of $O(4,2)$,

$$
\begin{aligned}
r &= \hat{L}_{56} - \hat{L}_{46}, \\
x^i &= \hat{L}_{i5} - \hat{L}_{i4}, \\
-i(\mathbf{x}\partial_{\mathbf{x}} + 1) &= \hat{L}_{45}, \\
-ir\partial_{x^i} &= \hat{L}_{i6}.
\end{aligned} \tag{54}
$$

The last equation follows from

$$
\partial_{x^i} = \frac{1}{2\vec{u}^2} e^i{}_\mu \partial_\mu, \tag{55}
$$

[see (185)], together with

$$u^1 = \frac{1}{2}(z_1 + z_1^*), \quad u^2 = \frac{1}{2i}(z_1 - z_1^*),$$
$$u^3 = \frac{1}{2}(z_2 + z_2^*), \quad u^4 = \frac{1}{2i}(z_2 - z_2^*), \tag{56}$$

and

$$\partial_1 = (\partial_{z_1} + \partial_{z_1^*}), \qquad \partial_2 = i(\partial_{z_1} - \partial_{z_1^*}),$$
$$\partial_3 = (\partial_{z_2} + \partial_{z_2^*}), \qquad \partial_4 = i(\partial_{z_2} - \partial_{z_2^*}). \tag{57}$$

Hence

$$-\,ir\partial_{x^i} = -\frac{i}{2}(\bar{z}\sigma_i\partial_{\bar{z}} + \partial_z\sigma_i z). \tag{58}$$

This is to be compared with the generators $\hat{L}_{AB}$ expressed in terms of the z, z^*'s,

$$\begin{aligned}
\hat{L}_{ij} &= \frac{1}{2}(\bar{z}\sigma_k\partial_{\bar{z}} - \partial_z\sigma_k z),\\
\hat{L}_{i4} &= -\frac{1}{2}(\bar{z}\sigma_i z - \partial_z\sigma_i\partial_{\bar{z}}),\\
\hat{L}_{i5} &= \frac{1}{2}(\bar{z}\sigma_i z + \partial_z\sigma_i\partial_{\bar{z}}),\\
\hat{L}_{i6} &= -\frac{i}{2}(\bar{z}\sigma_i\partial_{\bar{z}} + \partial_z\sigma_i z),\\
\hat{L}_{45} &= -\frac{i}{2}(\bar{z}\partial_{\bar{z}} + \partial_z z),\\
\hat{L}_{46} &= -\frac{1}{2}(\bar{z}z + \partial_z\partial_{\bar{z}}),\\
\hat{L}_{56} &= \frac{1}{2}(\bar{z}z - \partial_z\partial_{\bar{z}}).
\end{aligned} \tag{59}$$

From these we can also verify the other relations in (54). In fact, the generators L_{AB} can be expressed in terms of the x^i, ∂_{x^i} algebra as follows

$$\hat{L}_{ij} = -\frac{i}{2}(x^i\partial_{x^j} - x^j\partial_{x^i}),$$

$$
\begin{aligned}
\hat{L}_{i4} &= \frac{1}{2}\left(-x^i\partial_{\mathbf{x}}^2 - x^i + 2\partial_{x^i}\mathbf{x}\partial_{\mathbf{x}}\right), \\
\hat{L}_{i5} &= \frac{1}{2}\left(-x^i\partial_{\mathbf{x}}^2 + x^i + 2\partial_{x^i}\mathbf{x}\partial_{\mathbf{x}}\right), \\
\hat{L}_{i6} &= -ir\partial_{x^i}, \\
\hat{L}_{45} &= -i(\mathbf{x}\partial_{\mathbf{x}} + 1), \\
\hat{L}_{46} &= \frac{1}{2}(-r\partial_{\mathbf{x}}^2 - r), \\
\hat{L}_{56} &= \frac{1}{2}(-r\partial_{\mathbf{x}}^2 + r).
\end{aligned} \tag{60}
$$

where $\partial_{\mathbf{x}}^2$ and $\mathbf{x}\partial_{\mathbf{x}}$ are really $\partial_{x^\mu}^2$ and $x^\mu\partial_{x^\mu}$, being equal to the purely spatial sums only because of the constraint (29). When working with oscillator wave functions separated in the u^μ coordinates the convenient form of the generators is

$$
\begin{aligned}
\hat{L}_{12} &= i(u^1\partial_2 - u^2\partial_1 - u^3\partial_4 + u^4\partial_3)/2, \\
\hat{L}_{13} &= i(u^1\partial_3 + u^2\partial_4 - u^3\partial_1 - u^4\partial_2)/2, \\
\hat{L}_{14} &= -(u^1u^3 + u^2u^4) + (\partial_1\partial_3 + \partial_2\partial_4)/4, \\
\hat{L}_{15} &= (u^1u^3 + u^2u^4) + (\partial_1\partial_3 + \partial_2\partial_4)/4, \\
\hat{L}_{16} &= -i(u^1\partial_3 + u^2\partial_4 + u^3\partial_1 + u^4\partial_2)/2, \\
\hat{L}_{23} &= i(u^1\partial_4 - u^2\partial_3 + u^3\partial_2 - u^4\partial_1)/2, \\
\hat{L}_{24} &= -(u^1u^4 - u^2u^3) + (\partial_1\partial_4 - \partial_2\partial_3)/4, \\
\hat{L}_{25} &= (u^1u^4 + u^2u^3) + (\partial_1\partial_4 - \partial_2\partial_3)/4, \\
\hat{L}_{26} &= -i(u^1\partial_4 - u^2\partial_3 - u^3\partial_2 + u^4\partial_1)/2, \\
\hat{L}_{34} &= [(u^1)^2 + (u^2)^2 - (u^3)^2 - (u^4)^2]/2 + (\partial_1^2 + \partial_2^2 - \partial_3^2 - \partial_4^2)/8, \\
\hat{L}_{35} &= -[(u^1)^2 + (u^2)^2 - (u^3)^2 - (u^4)^2]/2 + (\partial_1^2 + \partial_2^2 - \partial_3^2 - \partial_4^2)/8, \\
\hat{L}_{36} &= -i(u^1\partial_1 + u^2\partial_2 - u^3\partial_3 - u^4\partial_4)/2, \\
\hat{L}_{45} &= -i(u^1\partial_1 + u^2\partial_2 + u^3\partial_3 + u^4\partial_4 + 2)/2, \\
\hat{L}_{46} &= -(u^\mu)^2/2 - \partial_\mu^2/8, \\
\hat{L}_{56} &= (u^\mu)^2/2 - \partial_\mu^2/8.
\end{aligned} \tag{61}
$$

The properly normalized H atom wave functions are

$$\psi_n^H(\mathbf{x}) = \frac{1}{\sqrt{n}} e^{i\vartheta_n \hat{D}} \psi_n^s(u^\mu) = \frac{1}{\sqrt{n}} \psi_n^s(u^\mu/\sqrt{n}). \tag{62}$$

They are orthonormal in the physical scalar product

$$\langle \psi'^{H}_{n'} | \psi^{H}_{n} \rangle_H = \langle \psi'^{s}_{n'} | (\hat{L}_{56} - \hat{L}_{46}) | \psi^{s}_{n} \rangle. \tag{63}$$

With this scalar product and the identifications (54) we can calculate the matrix elements of the dipole x^i and the momentum operator $-i\partial_{x^i}$ using only operations within the Lie algebra of the group $O(4,2)$. This is why $O(4,2)$ is called the *dynamical group* of the H atom system [1].

For completeness, let us mention that the relation between the physical states in the oscillator basis $|n_1 n_2 m\rangle^H$ and the usual eigenstates of fixed angular momentum $|nlm\rangle$ is given by the following linear combination

$$\psi_{nlm}(r,\vartheta,\varphi) = (-)^m \sum_{n_1+n_2+m=(n-1)/2} \sqrt{2l+1} \tag{64}$$
$$\times \begin{pmatrix} \frac{1}{2}(n-1) & \frac{1}{2}(n-1) & l \\ \frac{1}{2}(n_2-n_1+m) & \frac{1}{2}(n_1-n_2+m) & -m \end{pmatrix} \psi_{n_1 n_2 m}(\mathbf{x}).$$

The coefficients are the standard Wigner $3j$-symbols [9].

4 Path Integral

One of the most important successes of Schrödinger theory is the explanation of the energy levels and transition amplitudes of the hydrogen atom. Astonishingly, this fundamental system has resisted for many years all efforts to solve its path integral. The first essential structural ingredient was found in 1979 by Duru and Kleinert [3] by recognizing the need to work with a generalized pseudotime sliced path integral with a regulating function $f(\mathbf{x}) = r$. The detailed solution of the problem turned out to be much more subtle than originally expected. It required the understanding of path integrals in spaces with curvature and torsion [10] and will be presented here for the first time. In particular, we shall be careful in demonstrating the absence of any unwanted fluctuation corrections that have plagued all earlier attempts.

4.1 The Pseudotime Displacement Amplitude

Consider first the path integral for the time displacement amplitude of an electron proton system with H atom interactions. If m_e, m_p denotes the masses of the two particles with the reduced mass $M = m_e m_p/(m_e + m_p)$ and e the electron charge, the Hamiltonian reads

$$H = \frac{p^2}{2M} - \frac{e^2}{r}. \tag{65}$$

The formal expression for the amplitude

$$(\mathbf{x}_b t_b | \mathbf{x}_a t_a) = \int \mathcal{D}^3 x(t) \exp\left\{ \frac{i}{\hbar} \int_{t_b}^{t_a} dt(\mathbf{p}\dot{\mathbf{x}} - H) \right\} \tag{66}$$

cannot be time sliced into a finite number of integral since the path would collapse. It would stretch out into a straight line with $\dot{\mathbf{x}} \approx 0$ and slide down into the $1/r$ abyss. A stable path integral can be written down using the pseudotime displacement amplitude (12.32). A convenient family of regulating functions is

$$f_l(\mathbf{x}) = f(\mathbf{x})^{1-\lambda}, \quad f_r(\mathbf{x}) = f(\mathbf{x})^{\lambda}, \tag{67}$$

satisfying $f_l(\mathbf{x}) f_r(\mathbf{x}) = f(\mathbf{x}) = r$. With the path integral rooted in the general resolvent operator (12.25), all results must be independent of the splitting parameter λ after going to the continuum limit. This will be useful for a cross check of the calculations. Thus we shall consider the amplitude

$$\begin{aligned} \langle \mathbf{x}_b | \hat{\mathcal{U}}_E(S) | \mathbf{x}_a \rangle &= r_b^{\lambda} r_a^{1-\lambda} \int \mathcal{D}^D x(s) \int \frac{\mathcal{D}^D p(s)}{(2\pi\hbar)^D} \\ &\quad \times \exp\left\{ \frac{i}{\hbar} \int_0^S ds [\mathbf{p}\mathbf{x}' - r^{1-\lambda}(H - E) r^{\lambda}] \right\}, \end{aligned} \tag{68}$$

where the prime denotes the derivative with respect to the pseudotime argument s. For the sake of generality, we have allowed for a general dimension D of orbital motion. In the sliced form the amplitude reads

$$\begin{aligned} &\langle \mathbf{x}_b | \hat{\mathcal{U}}_E(S) | \mathbf{x}_a \rangle \approx r_b^{\lambda} r_a^{1-\lambda} \\ &\quad \times \prod_{n=2}^{N+1} \left[\int_{-\infty}^{\infty} d^D \Delta x_n \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{d^D p_n}{(2\pi\hbar)^D} \right] \exp\left\{ \frac{i}{\hbar} \mathcal{A}_E^N \right\}, \end{aligned} \tag{69}$$

with the action [using $\Delta \mathbf{x}_n \equiv \mathbf{x}_n - \mathbf{x}_{n-1}$, $\epsilon_s \equiv S/(N+1)$]

$$\mathcal{A}_E^N[\mathbf{p}, \mathbf{x}] = \sum_{n=1}^{N+1} \left[\mathbf{p}_n \, \Delta \mathbf{x}_n - \epsilon_s \, r_n^{1-\lambda} r_{n-1}^{\lambda} \left(\frac{\mathbf{p}_n^{\,2}}{2M} - E \right) + \epsilon_s \, e^2 \right]. \tag{70}$$

The last term carries initially a factor $(r_{n-1}/r_n)^\lambda$ which, however, is equal to unity in the continuum limit. Integrating out the momentum variables gives, after a convenient arrangement of the emerging $N{+}1$ factors $1/(r_n^{1-\lambda}\, r_{n-1}^\lambda)^{D/2}$, the configurational path integral

$$\langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle \approx \frac{r_b^\lambda r_a^{1-\lambda}}{\sqrt{2\pi\, i\epsilon_s\hbar\, r_b^{1-\lambda}\, r_a^\lambda/M}^D} \prod_{n=2}^{N+1}\left[\int \frac{d^D\Delta\mathbf{x}_n}{\sqrt{2\pi i\epsilon_s\hbar r_{n-1}/M}^D}\right] \times \exp\left\{\frac{i}{\hbar}\mathcal{A}_E^N[\mathbf{x},\mathbf{x}']\right\}, \tag{71}$$

with the pseudotime-sliced action

$$\mathcal{A}_E^N[\mathbf{x},\mathbf{x}'] = (N+1)\epsilon_s e^2 + \sum_{n=1}^{N+1}\left[\frac{M}{2}\frac{(\Delta\mathbf{x}_n)^2}{\epsilon_s r_n^{1-\lambda}\, r_{n-1}^\lambda} + \epsilon_s\, r_n E\right], \tag{72}$$

where we have replaced $r_n^{1-\lambda} r_{n-1}^\lambda$ by r_n since both have the same continuum limit. In this limit the action can formally be written as

$$\mathcal{A}_E[\mathbf{x},\mathbf{x}'] = e^2\, S + \int_0^S ds\left(\frac{M}{2r}\mathbf{x}'^2 + Er\right). \tag{73}$$

We shall treat this path integral first in the case $D=2$ where the movement of the electron is restricted to a plane and proceed afterwards to the physical case $D=3$. The case of general D is treated in Chapter 14 of the textbook [2].

4.2 Solution for $D = 2$ H atom System

First we observe that the kinetic pseudoenergy has scale dimensions $[rp^2] \sim [r^{-1}]$ which is precisely opposite to that of the potential term, $[r^{+1}]$. This is the same dimensional situation as in the harmonic oscillator, where the dimensions are $[p^2]=[r^{-2}]$ and $[r^{+2}]$, respectively. We therefore decide to go over to "square root coordinates" via some transformation which changes $r \to u^2$ [11]. In two dimensions, the appropriate square root is given by the Levi-Cività transformation

$$\begin{aligned} x^1 &= (u^1)^2 - (u^2)^2, \\ x^2 &= 2u^1 u^2. \end{aligned} \tag{74}$$

We may imagine the vectors $\mathbf{x}, \mathbf{u}$ to move in the complex planes $x = x^1 + ix^2$, $u = u^1 + iu^2$. Then the new variables u corresponds to the complex square root,

$$u = \sqrt{x}. \tag{75}$$

Let us also introduce the matrix

$$A(\mathbf{u}) = \begin{pmatrix} u^1 & -u^2 \\ u^2 & u^1 \end{pmatrix}, \tag{76}$$

and write (74) as a matrix equation

$$\mathbf{x} = A\mathbf{u}. \tag{77}$$

In contrast to the three-dimensional case to be treated below we note here the rather obvious fact that the Levi-Cività mapping, which is simply a transformation to parabolic coordinates, carries the flat x^i space into a flat u^μ space. Indeed, from (74) we have the infinitesimal transformation $dx^i = e^i{}_\mu(\mathbf{u})\, du^\mu$ with the basis dyad

$$e^i{}_\mu(\mathbf{u}) = \frac{\partial x^i}{\partial u^\mu} = 2A^i{}_\mu(\mathbf{u}), \tag{78}$$

and the reciprocal dyad

$$e_i{}^\mu(\mathbf{u}) = \frac{1}{2} A^{-1T}{}_i{}^\mu = \frac{1}{2\mathbf{u}^2} A^i{}_\mu(\mathbf{u}). \tag{79}$$

We therefore find for the connection,

$$\Gamma_{\mu\nu}{}^\lambda = e_i{}^\lambda\, \partial_\mu\, e^i{}_\nu, \tag{80}$$

the matrix elements $(\Gamma_\mu)_\nu{}^\lambda$ as follows

$$\begin{aligned} (\Gamma_1)_\mu{}^\nu &= \frac{1}{\mathbf{u}^2} \begin{pmatrix} u^1 & -u^2 \\ u^2 & u^1 \end{pmatrix}_\mu{}^\nu = \frac{1}{2\mathbf{u}^2} A(\mathbf{u})^\mu{}_\nu, \\ (\Gamma_2)_\mu{}^\nu &= \frac{1}{\mathbf{u}^2} \begin{pmatrix} u^2 & u^1 \\ -u^1 & u^2 \end{pmatrix}_\mu{}^\nu. \end{aligned} \tag{81}$$

Notice that the connection satisfies an important identity

$$\Gamma_\mu{}^{\mu\nu} \equiv 0, \tag{82}$$

which is seen to be a consequence of the defining relation

$$\Gamma_\mu{}^{\mu\nu} \equiv g^{\mu\nu} e_i{}^\lambda \partial_\mu e^i{}_\nu, \tag{83}$$

together with the obvious identity

$$\partial_\mu e^i{}_\mu = 0, \tag{84}$$

and the diagonal property of $g^{\mu\nu} = \delta^{\mu\nu}/4r$. It can be shown quie generally that this is the essential reason for the absence of the time slicing corrections to be proved in this section.

Both, torsion and Cartan curvature tensor vanish identically, the latter due to the linearity of the basis dyads $e^i{}_\mu(\mathbf{u})$ in $\mathbf{u}$, which guarantees trivially the integrability conditions

$$e_i{}^\lambda (\partial_\mu e^i{}_\nu - \partial_\nu e^i{}_\mu) \equiv 0, \tag{85}$$

$$e_i{}^\kappa (\partial_\mu \partial_\nu - \partial_\nu \partial_\mu) e^i{}_\lambda \equiv 0, \tag{86}$$

and thus $S_{\mu\nu}{}^\lambda \equiv 0$, $R_{\mu\nu\lambda}{}^\kappa \equiv 0$. In the continuum limit it is easy to see that the Levy-Cività transformation converts the action (73) into that of a harmonic oscillator. With

$$\mathbf{x}'^2 = 4\mathbf{u}^2\, \mathbf{u}'^2 = 4r\, \mathbf{u}'^2 \tag{87}$$

we find

$$\mathcal{A}[\mathbf{x}, \mathbf{x}'] = e^2 S + \int_0^S ds \left(\frac{4M}{2} \mathbf{u}'^2 + E\mathbf{u}^2 \right). \tag{88}$$

Apart from the trivial term $e^2 S$, this is the action of a harmonic oscillator,

$$\mathcal{A}_{os}[\mathbf{u}, \mathbf{u}'] = \int_0^S ds \frac{\mu}{2} (\mathbf{u}'^2 - \omega^2 \mathbf{u}^2), \tag{89}$$

which oscillates in the pseudotime s with an effective mass

$$\mu = 4M, \tag{90}$$

and a pseudofrequency

$$\omega = \sqrt{-E/2M}. \tag{91}$$

Note that this ω has the same dimension as 1/pseudotime s corresponding to $[\omega] = [r/t]$ (in contrast to usual frequencies with $[1/t]$).

The path integral is well defined only as long as the energy E of the H atom is negative, i.e., in the bound-state regime. The amplitude in the continuum regime with positive E will be obtained by analytic continuation.

In the regularized form we can now calculate the pseudotime sliced amplitude. Taking for the splitting parameter $\lambda = 1/2$ and ignoring, for a moment, all complications due to the finite time slicing, we deduce from (66),

$$d\mathbf{x} = 2A(\mathbf{u})d\mathbf{u}, \tag{92}$$

and hence

$$d^2x_n = 4\mathbf{u}_n{}^2 d^2u_n. \tag{93}$$

Writing the integrals over the $\Delta\mathbf{x}_n$'s in (71) as integrals over $\mathbf{x}_n$'s we see that the transformed amplitude (71) becomes simply

$$\langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle = \frac{1}{4}e^{ie^2S/\hbar}[(\mathbf{u}_bS|\mathbf{u}_a0) + (-\mathbf{u}_bS|\mathbf{u}_a0)], \tag{94}$$

where $(\mathbf{u}_bS|\mathbf{u}_a0)$ denotes the time sliced oscillator amplitude

$$(\mathbf{u}_bS|\mathbf{u}_a0) \approx \frac{1}{2\pi i\hbar\epsilon_s/\mu}\prod_{n=1}^{N}\left[\int\frac{d^2u_n}{2\pi i\hbar\epsilon_s/\mu}\right] \times\exp\left\{\frac{i}{\hbar}\sum_{n=1}^{N}\frac{\mu}{2}\left(\frac{1}{\epsilon_s}\Delta\mathbf{u}_n{}^2 - \epsilon_s\omega^2\mathbf{u}_n{}^2\right)\right\} \tag{95}$$

The integrals can all be done with the known result, in the limit $N\to\infty$,

$$(\mathbf{u}_bS|\mathbf{u}_a0) = \frac{\mu\omega}{2\pi i\hbar\sin\omega S}\exp\left\{\frac{i}{\hbar}\frac{\mu\omega}{\sin\omega S}[(\mathbf{u}_b{}^2+\mathbf{u}_a{}^2)\cos\omega S - 2\mathbf{u}_b\mathbf{u}_a]\right\}. \tag{96}$$

The symmetrization in $\mathbf{u}_b$ in (94) is necessary since for each path from $\mathbf{x}_a$ to $\mathbf{x}_b$ there are two paths in the square-root space, one from $\mathbf{u}_a$ to $\mathbf{u}_b$ and one from $\mathbf{u}_a$ to $-\mathbf{u}_b$.

The fixed-energy amplitudes are obtained by integrating the pseudotime displacement amplitude over all S.

$$(\mathbf{x}_b|\mathbf{x}_a)_E = \int_0^\infty dS\, e^{ie^2S/\hbar}\,\frac{1}{4}[(\mathbf{u}_bS|\mathbf{u}_a0) + (-\mathbf{u}_bS|\mathbf{u}_a0)]. \tag{97}$$

Inserting (96), this becomes

$$(\mathbf{x}_b|\mathbf{x}_a)_E = \frac{1}{2}\int_0^\infty dS \exp(ie^2 S/\hbar) F^2(S)$$
$$\times \exp\left[-\pi F^2(S)(\mathbf{u}_b^2 + \mathbf{u}_a^2)\cos\omega S\right]\ \cosh\left[2\pi F^2(S)\mathbf{u}_b\mathbf{u}_a\right], \tag{98}$$

with the abbreviation

$$F(S) = \sqrt{\mu\omega/2\pi i\hbar \sin\omega S}, \tag{99}$$

which is the one-dimensional fluctuation factor [see (2.145)]. The $\mathbf{u}$'s on the right-hand side are related to the $\mathbf{x}$'s on the left by

$$\mathbf{u}_{a,b}^2 = r_{a,b}, \quad \mathbf{u}_b\mathbf{u}_a = \sqrt{(r_b r_a + \mathbf{x}_b\mathbf{x}_a)/2}. \tag{100}$$

In doing the integral we have to circumnavigate the singularities in $F(S)$ in accordance with the $i\eta$-prescription $\omega \to \omega - i\eta$. This can be avoided by rotating the contour of S-integration so that it runs along the negative imaginary semi-axis,

$$S = -i\sigma, \quad \sigma \in (0, \infty).$$

This amounts to going over to the euclidean amplitude of the harmonic oscillator. The amplitude can be rewritten in a pleasant form by introducing further the variables

$$\varrho \equiv e^{-2i\omega S} = e^{-2\omega\sigma}, \tag{101}$$

$$\kappa \equiv \frac{\mu\omega}{2\hbar} = \frac{2M\omega}{\hbar} = \sqrt{-2ME/\hbar^2},$$

$$\nu \equiv \frac{e^2}{2\omega\hbar} = \sqrt{\frac{e^4 M}{-2\hbar^2 E}}. \tag{102}$$

Then

$$\pi F^2(S) = \kappa\frac{2\sqrt{\varrho}}{1-\varrho}, \tag{103}$$

$$e^{ie^2 s/\hbar} F^2(S) = \frac{2}{\pi}\kappa\frac{\varrho^{1/2-\nu}}{1-\varrho}, \tag{104}$$

and we obtain

$$(\mathbf{x}_b|\mathbf{x}_a)_E = -i\frac{M}{\pi\hbar}\int_0^1 d\varrho \frac{\varrho^{-1/2-\nu}}{1-\varrho}\cos\left\{2\kappa\frac{2\sqrt{\varrho}}{1-\varrho}\sqrt{(r_br_a+\mathbf{x}_b\mathbf{x}_a)/2}\right\}$$
$$\times \exp\left\{-\kappa\frac{1+\varrho}{1-\varrho}(r_b+r_a)\right\}. \qquad (105)$$

This can be used to find the energy spectrum and the wave functions.

Notice that the integral converges only for $\nu < 1/2$. It is possible to write down another integral representation which converges for all $\nu \neq 1/2, 3/2, 5/2, \dots$. For this we change the variables of integration to

$$\zeta \equiv \frac{1+\varrho}{1-\varrho}, \quad \zeta - 1 = \frac{2\varrho}{1-\varrho}, \quad \zeta+1 = \frac{2}{1-\varrho}, \qquad (106)$$

so that

$$\frac{d\varrho}{(1-\varrho)^2} = \frac{1}{2}d\zeta, \quad \varrho = \frac{\zeta-1}{\zeta+1}. \qquad (107)$$

This gives

$$(\mathbf{x}_b|\mathbf{x}_a)_E = -i\frac{M}{\pi\hbar}\frac{1}{2}\int_1^\infty d\zeta(\zeta-1)^{-\nu-1/2}(\zeta+1)^{\nu-1/2}$$
$$\times \cos\left\{2\kappa\sqrt{\zeta^2-1}\sqrt{(r_br_a+\mathbf{x}_b\mathbf{x}_a)/2}\right\} e^{-\kappa\zeta(r_b+r_a)}. \qquad (108)$$

The integrand has a cut in the complex ζ-plane from $z = -1$ to $-\infty$ and from $\zeta = 1$ to ∞, with the integral running along the right-hand cut. This is transformed into an integral along a contour C which encircles the right-hand cut in the clockwise sense. Since the cut is of the type $(\zeta-1)^{-\nu-1/2}$, we have the replacement rule

$$\int_1^\infty d\zeta(\zeta-1)^{-\nu-1/2}\dots \to \frac{\pi e^{i\pi(\nu+1/2)}}{\sin[\pi(\nu+1/2)]}\frac{1}{2\pi i}\int_C d\zeta(\zeta-1)^{-\nu-1/2}\dots\,, \qquad (109)$$

and obtain

$$(\mathbf{x}_b|\mathbf{x}_a)_E = -i\frac{M}{\pi\hbar}\frac{1}{2}\frac{\pi e^{i\pi(\nu+1/2)}}{\sin[\pi(\nu+1/2)]}\int_C \frac{d\zeta}{2\pi i}(\zeta-1)^{-\nu-1/2}(\zeta+1)^{\nu-1/2}$$
$$\times \cos\left\{2\kappa\sqrt{\zeta^2-1}\sqrt{(r_br_a+\mathbf{x}_b\mathbf{x}_a)/2}\right\} e^{-\kappa\zeta(r_b+r_a)}. \qquad (110)$$

4.3 Solution for $D = 3$ H atom

After the two-dimensional exercise we now turn to the physically relevant H atom in three dimensions. We have to find again some kind of "square-root" coordinates which convert the potential $-Er$ in the pseudotime Hamiltonian in the action of the amplitude (68) into a harmonic potential. In two dimensions the answer was a complex square-root. Here it will be a "quaternionic square-root", i.e., the *Kustaanheimo-Stiefel transformation*. In the path intergral, we now incorporate the dummy forth dimension into the action by replacing, in the kinetic term, $\mathbf{x}$ by $\vec{x}$ and extending the kinetic action to

$$\mathcal{A}_{kin}^N \equiv \sum_{n=1}^{N+1} \frac{M}{2} \frac{(\vec{x}_n - \vec{x}_{n-1})^2}{\epsilon_s r_n^{1-\lambda} r_{n-1}^{\lambda}}. \tag{111}$$

The additional contribution of the forth components $x_n^4 - x_{n-1}^4$ can be eliminated trivially from the final pseudotime displacement amplitude by integrating each time slice over dx_n^4 with the measure

$$\prod_{n=1}^{N+1} \int_{-\infty}^{\infty} \frac{d(x^4)_{n-1}}{\sqrt{2\pi i \epsilon_s \hbar r_n^{1-\lambda} r_{n-1}^{\lambda}/M}}. \tag{112}$$

In contrast to the spatial $d^3 x_n{}'$s, the forth coordinate is integrated also over the initial slice variable x_0^4. Then we have the trivial identity

$$\prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{d(\Delta x^4)_{n-1}}{\sqrt{2\pi i \epsilon_s \hbar r_n^{1-\lambda} r_{n-1}^{\lambda}/M}} \right] \exp\left\{ \frac{i}{\hbar} \sum_{n=1}^{N+1} \frac{M}{2} \frac{(\Delta x_n^4)^2}{\epsilon_s r_n^{1-\lambda} r_{n-1}^{\lambda}} \right\} = 1. \tag{113}$$

This allows to extend the path integral by the dummy forth component of the orbits, $x^4(t)$, without changing the amplitude. Thus we arrive at the formula

$$\begin{aligned} \langle \mathbf{x}_b | \hat{\mathcal{U}}_E(S) | \mathbf{x}_a \rangle \;\; &= \int dx_a^4 \frac{r_b^{\lambda} r_a^{1-\lambda}}{(2\pi i \epsilon_s \hbar r_b^{1-\lambda} r_a^{\lambda}/M)^2} \\ &\times \prod_{n=2}^{N+1} \left[\int_{-\infty}^{\infty} \frac{d^4 \Delta x_n}{(2\pi i \epsilon_s \hbar r_{n-1}/M)^2} \right] \exp\left\{ \frac{i}{\hbar} \mathcal{A}_E^N \right\}, \end{aligned} \tag{114}$$

where $\mathcal{A}_E^N$ is now the action (72) but with the three-vectors $\mathbf{x}_n$ replaced by four vectors $\vec{x}_n$ (while r is still the length of the spatial part of $\vec{x}$). Distributing the r_b, r_n, r_a factors evenly over the intervals and shifting the r_n's in the denominators to r_{n+1}'s, following the same procedure as in Eq. (156), we arrive at the pseudotime displacement amplitude

$$\langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle = \frac{1}{(2\pi\, i\epsilon_s\hbar/M)^2}\int_{-\infty}^{\infty}\frac{dx_a^4}{r_a} \times\prod_{n=2}^{N+1}\left[\int\frac{d^4\Delta\vec{x}_n}{(2\pi i\epsilon_s\hbar r_n^2/M)^2}\right]\exp\left\{\frac{i}{\hbar}(\mathcal{A}_E^N+\mathcal{A}_f^N)\right\}, \tag{115}$$

with the sliced action

$$\mathcal{A}_E^N[\vec{x},\vec{x}'] = (N+1)\epsilon_s e^2 + \sum_{n=1}^{N+1}\left[\frac{M}{2}\frac{(\Delta\vec{x}_n)^2}{\epsilon_s r_n^{1-\lambda}\, r_{n-1}^{\lambda}} + \epsilon_s\, r_n^{1-\lambda}\, r_{n-1}^{\lambda}\, E\right]. \tag{116}$$

The action $\mathcal{A}_f^N$ is again due to the remaining prefactors, which are now $(r_b/r_a)^{3\lambda-2} = \prod_1^{N+1}(r_n/r_{n-1})^{3\lambda-2}$, so that we have, after a shift of the denominators $1/r_{n-1}^2$ to $1/r_n^2$, which changes the power $3\lambda-2$ to 3λ [compare (158)],

$$\frac{i}{\hbar}\mathcal{A}_f^N = 3\lambda\sum_{n=1}^{N+1}\log\left(\frac{\vec{u}_n^2}{\vec{u}_{n-1}^2}\right). \tag{117}$$

As in the two-dimensional case we shall at first ignore the subtleties due to the time slicing. Thus we set $\lambda = 0$ and do the transformation formally on the continuum limit of the action $\mathcal{A}_E^N$, which looks the same as in (73). Using the properties of the matrix A in (15),

$$\begin{aligned} A^T &= 4\vec{u}^2A^{-1}, \\ \det A &= \sqrt{\det(AA^T)} = 16r^2, \end{aligned} \tag{118}$$

we see that

$$\vec{x}'^2 = 4\vec{u}^2\vec{u}'^2 = 4r\vec{u}'^2, \tag{119}$$

and

$$d^4x = 16r^2d^4u. \tag{120}$$

In this way we find the formal relation

$$\langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle = e^{ie^2S/\hbar}\frac{1}{16}\int_{-\infty}^{\infty}\frac{dx_a^4}{r_a}(\vec{u}_bS|\vec{u}_a0), \tag{121}$$

where $(\vec{u}_b S|\vec{u}_a 0)$ is the time displacement amplitude of the four-dimensional harmonic oscillator,

$$(\vec{u}_b S|\vec{u}_a 0) = \int \mathcal{D}^4 u(s) \exp\left\{\frac{i}{\hbar}\mathcal{A}_{os}\right\}, \tag{122}$$

with the action

$$\mathcal{A}_{os} = \int_0^S ds \frac{\mu}{2}(\vec{u}'^2 - \omega^2 \vec{u}^2). \tag{123}$$

This is the analog of Eq. (94). The parameters are

$$\begin{aligned} \mu &= 4M, \\ \omega &= \sqrt{-E/2M}, \end{aligned} \tag{124}$$

just as in (90) and (91). The integral $\int dx_a^4/r_a$ can be rewritten as an integral over the third Euler angle γ using the relation (16). Since $\mathbf{x}$ and thus the polar angles θ, φ are kept fixed during the integration, we have directly $\int dx_a^4/r_a = \int d\alpha_a$. As far as the range of integration is concerned we note that it should be taken only over a single period $\gamma_a \in [0, 4\pi]$, The other periods are conventionally included in the oscillator amplitude. When specifying a four-vector $\vec{u_b}$, all paths have to been summed to the final Euler angle γ_b and to all its periodic repetitions which by (9) have the same $\vec{u_b}$. The sum over initial periods appearing in (121) is of course completely equivalent to this. As it stands, the oscillator amplitude on the right-hand side of (121) has to be understood as referring to the extended zone scheme in the Euler angle γ used in specifying $\vec{u}$. In the reduced zone scheme which is in use when specifying $\vec{u}_b, \vec{u}_a$, we should rewrite (121) correctly as

$$\langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle = e^{ie^2 S/\hbar}\frac{1}{16}\int_0^{4\pi} d\gamma_a (\vec{u}_b S|\vec{u}_a 0). \tag{125}$$

The reason why the other periods in (121) must be omitted can also be understood by comparison with the two-dimensional case. There we had observed a two-fold degeneracy of contributions to the time sliced path integral which cancelled all factors 2 in the measure (160). Here the same thing happens but with an infinite degeneracy: When integrating over all images d^4u_n of d^4x_n in the oscillator

path integral we cover the original $\mathbf{x}$-space once for $\gamma_n \in [0, 4\pi]$ and repeat doing so for each further period $\gamma_n \in [4\pi l, 4\pi(l+1)]$. Therefore, each volume element d^4u_n really has to be divided by an infinite factor to remove this degeneracy. This, however, is not necessary since the gradient term compensates precisely the same infinite factor. Indeed,

$$(\vec{u}_n + \vec{u}_{n-1})^2(\vec{u}_n - \vec{u}_{n-1})^2 \tag{126}$$

is small for $\vec{x}_n \approx \vec{x}_{n-1}$ at infinitely many places of $\gamma_n - \gamma_{n-1}$, once in each periodic repetition of the interval $[0, 4\pi]$. The infinite degeneracy cancels the infinite factor in the denominator of the measure. The only place where there is no such cancellation is in the integration $\int dx_a^4/r_a$. Here the infinite factor in the denominator is still present and is taken into account by integrating γ_a only over a single period. This is why (134) is the correct fixed-energy amplitude.

Notice that a shift of γ_a by a half-period 2π changes $\vec{u}$ to $-\vec{u}$ and thus corresponds to the two-fold degeneracy in the two-dimensional system.

The time sliced path integral for the harmonic oscillator can immediately be done, the amplitude being the four-dimensional version of (96),

$$\begin{aligned}(\vec{u}_b S|\vec{u}_a 0) &= \frac{1}{(2\pi i\hbar\epsilon_s/\mu)^2}\prod_{n=1}^{N}\left[\int\frac{d^4\Delta u_n}{2\pi i\hbar\epsilon_s/\mu}\right]\\ &\quad\times\exp\left\{\frac{i}{\hbar}\sum_{n=1}^{N}\frac{\mu}{2}\left(\frac{1}{\epsilon_s}\Delta\vec{u}_n{}^2 - \epsilon_s\omega^2\vec{u}_n^2\right)\right\} \qquad (127)\\ &= \frac{\omega^2}{(2\pi i\hbar\sin\omega S\,/\mu)^2}\exp\left\{\frac{i}{\hbar}\frac{\mu\omega}{\sin\omega S}[(\vec{u}_b{}^2+\vec{u}_a^2)\cos\omega S - 2\vec{u}_b\vec{u}_a]\right\}.\end{aligned}$$

To find the fixed-energy amplitude we have to integrate this over S:

$$(\mathbf{x}_b|\mathbf{x}_a)_E = \int_0^\infty dS e^{ie^2S/\hbar}\frac{1}{16}\int_0^{4\pi}d\gamma_a(\vec{u}_b S|\vec{u}_a 0). \tag{128}$$

Just as in (98), the integral is written most conveniently in terms of the variables (101), (102), so that we obtain for the fixed-energy amplitude of the three-dimensional H atom

$$\begin{aligned}(\mathbf{x}_b|\mathbf{x}_a)_E &= \frac{1}{16}\int_0^\infty dS e^{ie^2S/\hbar}\int_0^{4\pi}d\gamma_a(\vec{u}_b s|\vec{u}_a\ 0)\\ &= -i\frac{\omega M^2}{2\pi^2\hbar^2}\int_{-\infty}^{\infty}\frac{dx_a^4}{r_a}\int_0^1 d\varrho\frac{\varrho^{-\nu}}{(1-\varrho)^2} \qquad (129)\\ &\quad\times\exp\left\{2\kappa\frac{2\sqrt{\varrho}}{1-\varrho}\vec{u}_b\vec{u}_a\right\}\exp\left\{-\kappa\frac{1+\varrho}{1-\varrho}(r_b+r_a)\right\}.\end{aligned}$$

To do the integral over dx_b^4 we now express $\vec{u}_b\vec{u}_a$ in terms of the polar angles and find

$$\begin{aligned}
\vec{u}_b\vec{u}_a &= \sqrt{r_b r_a}\,\{\cos(\theta_b/2)\cos(\theta_a/2)\cos[(\varphi_b-\varphi_a+\gamma_b-\gamma_a)/2] \\
&\qquad +\sin(\theta_b/2)\sin(\theta_a/2)\cos[(\varphi_b-\varphi_a-\gamma_b+\gamma_a)/2]\} \\
&= \sqrt{r_b r_a}\,\{\cos[(\theta_b-\theta_a)/2]\cos[(\varphi_b-\varphi_a)/2]\cos[(\gamma_b-\gamma_a)/2] \\
&\qquad -\cos[(\theta_b+\theta_a)/2]\sin[(\varphi_b-\varphi_a)/2]\sin[(\gamma_b-\gamma_a)/2]\}\,.
\end{aligned} \tag{130}$$

This can be rewritten as

$$\vec{u}_b\vec{u}_a = \sqrt{(r_b r_a+\mathbf{x}_b\mathbf{x}_a)/2}\,\cos[(\gamma_b-\gamma_a+\beta)/2], \tag{131}$$

where β is the angle with

$$\tan\frac{\beta}{2} = \frac{\cos[(\theta_b+\theta_a)/2]\sin[(\varphi_b-\varphi_a)/2]}{\cos[(\theta_b-\theta_a)/2]\cos[(\varphi_b-\varphi_a)/2]}, \tag{132}$$

and

$$\cos\frac{\beta}{2} = \cos\frac{\theta_b-\theta_a}{2}\cos\frac{\varphi_b-\varphi_a}{2}\frac{r_b r_a}{\sqrt{(r_b r_a+\mathbf{x}_b\mathbf{x}_a)/2}}. \tag{133}$$

The integral $\int_0^{4\pi} d\gamma_a$ can now be done at each fixed $\mathbf{x}$. This gives [3, 12]

$$\begin{aligned}
(\mathbf{x}_b|\mathbf{x}_a)_E &= -i\frac{M\kappa}{\pi\hbar}\int_0^1 d\varrho\frac{\varrho^{-\nu}}{(1-\varrho)^2}I_0\left(2\kappa\frac{2\sqrt{\varrho}}{1-\varrho}\sqrt{(r_b r_a+\mathbf{x}_b\mathbf{x}_a)/2}\right) \\
&\qquad \times\exp\left\{-\kappa\frac{1+\varrho}{1-\varrho}(r_b+r_a)\right\},
\end{aligned} \tag{134}$$

where κ and ν are the same parameters as in Eq. (102).

In analogy with the two-dimensional case we observe that the integral converges only for $\nu < 1$. It is possible to write down another integral represention which converges for all $\nu \neq 1,2,3,\dots$. by changing again the variables of integration to $\zeta \equiv (1+\varrho)/(1-\varrho)$, and transform the integral over ζ into a contour integral encircling the cut from $\zeta = 1$ to ∞ in the clockwise sense. Since the cut is now of the type $(\zeta-1)^{-\nu}$, we have the replacement rule

$$\int_1^\infty d\zeta(\zeta-1)^{-\nu}\dots \to \frac{\pi e^{i\pi\nu}}{\sin\pi\nu}\int_C\frac{d\zeta}{2\pi i}(\zeta-1)^{-\nu}\dots\ . \tag{135}$$

Thus we obtain

$$(\mathbf{x}_b|\mathbf{x}_a)_E = -i\frac{M}{\pi\hbar}\frac{\kappa}{2}\frac{\pi e^{i\pi\nu}}{\sin\pi\nu}\int_C \frac{d\zeta}{2\pi i}(\zeta-1)^{-\nu}(\zeta+1)^{\nu}$$
$$\times I_0(2\kappa\sqrt{\zeta^2-1}\sqrt{(r_br_a+\mathbf{x}_b\mathbf{x}_a)/2})e^{-\kappa\zeta(r_b+r_a)}. \quad (136)$$

4.4 Absence of Time Slicing Corrections

We shall now convince ourselves that the finite thickness of the pseudotime slices does not change the above results. For this it is essential to make use of the correct measure for the path integral in a space with curvature and torsion. This is ruled by the new *quantum equivalent principle* (QEP) published only recently [8].

4.4.1 Measure of Path Integral in Space with Curvature and torsion

To avoid repeating the discussion of [8] we only quote here the result.

The QEP states that if cartesian coordinates x^i are transformed nonholonomically into a space with curvature and torsion parametrized by q^μ via

$$dx^i = e^i{}_\mu dq^\mu \quad (137)$$

with some basis n-ade e^i_μ, the time-sliced path integral measure $\prod d\Delta x^i_n$ goes over into

$$\prod_n d\Delta x^i_n = \prod_n d\Delta q^\mu_n \sqrt{g(q^\mu_n)}e^{i\sum_n \mathcal{A}^\epsilon_J/\hbar} \quad (138)$$

with an action coming from the Jacobian between Δx^i_n and Δq^μ_n:

$$\frac{i}{\hbar}\mathcal{A}^\epsilon_J = -e_i{}^\kappa e^i{}_{\kappa,\nu}\Delta q^\nu + \frac{1}{2}[e_i{}^\mu e^i_{\{\mu,\nu\lambda\}} - e_i{}^\mu e^i_{\{\kappa,\nu\}}e_j{}^\kappa e^j{}_{\{\mu,\lambda\}}]\Delta q^\nu\Delta q^\lambda$$
$$= -\Gamma_{\{\nu\mu\}}{}^\mu\Delta q^\nu \quad (139)$$
$$+\frac{1}{2}[\partial_{\{\mu}\Gamma_{\nu,\kappa\}}{}^\kappa + \Gamma_{\{\nu,\kappa}{}^\sigma\Gamma_{\mu\},\sigma}{}^\kappa - \Gamma_{\{\nu\kappa\}}{}^\sigma\Gamma_{\{\mu,\sigma\}}{}^\kappa]\Delta q^\nu\Delta q^\mu.$$

We have omitted the subscripts n of $\Delta q^\mu_n = q^\mu_n - q^\mu_{n-1}$ and the (postpoint) arguments of the coefficients q^μ_n, for brevity.

4.4.2 $D = 2$

With the above measure we can now easily convince ourselves that the finite thickness of the pseudotime slices does not change the above results. For the potential term this is obvious since it is of order ϵ_s and the time slicing can only produce higher than linear terms in ϵ_s which do not contribute in the continuum limit $\epsilon_s \to 0$. The crucial point where corrections could enter is in the transformation of the measure and the pseudotime-sliced kinetic terms in (71), (72). In vector notation, the coordinates transformation reads, at every time slice n,

$$\mathbf{x}_n = A(\mathbf{u}_n)\mathbf{u}_n. \tag{140}$$

Since this relation is quadratic in $\mathbf{u}$ we find the transformation of the coordinate differences

$$\Delta\mathbf{x}_n = 2A(\bar{\mathbf{u}}_n)\Delta\mathbf{u}_n, \tag{141}$$

and from this

$$(\Delta\mathbf{x}_n)^2 = 4\bar{\mathbf{u}}_n^2(\Delta\mathbf{u}_n)^2, \tag{142}$$

where $\bar{\mathbf{u}}_n$ is average across the slice

$$\bar{\mathbf{u}}_n \equiv (\mathbf{u}_n + \mathbf{u}_{n-1})/2. \tag{143}$$

Eq. (142) replaces the continuum relation (87). The sliced kinetic terms are therefore

$$\sum_{n=1}^{N+1} \frac{(\Delta\mathbf{x}_n)^2}{2\epsilon_s r_n^{1-\lambda} r_{n-1}^{\lambda}} = \sum_{n=1}^{N+1} \frac{4\bar{\mathbf{u}}_n^2}{2\epsilon_s(\mathbf{u}_n^2)^{1-\lambda}(\mathbf{u}_{n-1}^2)^{\lambda}}(\Delta\mathbf{u}_n)^2. \tag{144}$$

We now expand each of the gradient terms around the upper point of support, the postpoint, i.e.,

$$\begin{aligned}
\bar{\mathbf{u}}_n &= \mathbf{u}_n - \frac{1}{2}\Delta\mathbf{u}_n, && (145)\\
\mathbf{u}_{n-1} &= \mathbf{u}_n - \Delta\mathbf{u}_n, && (146)\\
\frac{\bar{\mathbf{u}}_n^2}{(\mathbf{u}_n^2)^{1-\lambda}(\mathbf{u}_{n-1}^2)^{\lambda}} &= 1 + (2\lambda - 1)\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_{n-1}^2} + \left(\frac{1}{4} - \lambda\right)\frac{{\Delta\mathbf{u}_n}^2}{\mathbf{u}_n^2}\\
&\quad +2\lambda^2\left(\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2}\right)^2. && (147)
\end{aligned}$$

It is useful to separate the gradient part of the action into a leading term

$$\mathcal{A}_0^\epsilon(\Delta\mathbf{u}_n) = 4M\frac{(\Delta\mathbf{u}_n)^2}{2\epsilon_s}, \tag{148}$$

plus a correction term

$$\begin{aligned}\Delta\mathcal{A}^\epsilon = {} & 4M\frac{(\Delta\mathbf{u}_n)^2}{2\epsilon_s} \\ & \times\left[(2\lambda-1)\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2} + \left(\frac{1}{4}-\lambda\right)\frac{\Delta\mathbf{u}_n{}^2}{\mathbf{u}_n^2} + 2\lambda^2\left(\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2}\right)^2\right].\end{aligned} \tag{149}$$

To calculate the proper transformation of the measure of integration in (71) we take

$$e^i{}_\mu(\mathbf{u}) = 2A^i{}_\mu(\mathbf{u}). \tag{150}$$

and insert it into the transformation law (138), (139). In the present case the terms involving two derivatives of $e^i{}_\mu$ are absent due to the purely quadratic nature of (150) in Δu^μ. The Jacobian action is therefore given by the shorter expressions

$$\begin{aligned}\frac{i}{\hbar}\mathcal{A}_J^\epsilon &= -e_i{}^\mu e^i{}_{\{\mu,\nu\}}\Delta u^\nu - \frac{1}{2}e_i{}^\mu e^i{}_{\{\kappa,\nu\}}e_j{}^\kappa e^j{}_{\mu,\lambda}\Delta u^\nu\Delta u^\lambda \\ &= -\Gamma_{\{\nu\mu\}}{}^\mu\Delta u^\nu - \frac{1}{2}\Gamma_{\{\nu\kappa\}}{}^\mu\Gamma_{\{\mu\lambda\}}{}^\kappa\Delta u^\nu\Delta u^\lambda.\end{aligned} \tag{151}$$

The coefficients are easily calculated using the reciprocal basis dyad,

$$e_i{}^\kappa = \frac{1}{2\mathbf{u}^2}e^i{}_\kappa, \tag{152}$$

as

$$\begin{aligned}\Gamma_{\nu\mu}{}^\mu &= e_i{}^\mu\partial_\nu e^i{}_\mu = \frac{2u^\nu}{\mathbf{u}^2}, \\ \Gamma_{\mu\nu}{}^\mu &= -e^i{}_\nu\partial_\mu e_i{}^\mu = \frac{2u^\nu}{\mathbf{u}^2}, \\ \Gamma_{\nu\kappa}{}^\sigma\Gamma_{\lambda\sigma}{}^\kappa &= -\partial_\lambda e_i{}^\kappa\partial_\nu e^i{}_\kappa = -\frac{2}{\mathbf{u}^4}(\delta^{\nu\lambda}\mathbf{u}^2 - 2u^\nu u^\lambda).\end{aligned} \tag{153}$$

The second equation is found directly from

$$- \partial_\mu e_i{}^\mu = -\partial_\mu (2\mathbf{u}^2)^{-1} e^i{}_\mu = e_i{}^\mu \; 2u^\mu \mathbf{u}^{-2}. \tag{154}$$

This, in turn, follows from the obvious identity $\partial_\mu e^i{}_\mu = 0$. Notice that the third expression is automatically equal to $\Gamma_{\{\nu\kappa\}}{}^\sigma \Gamma_{\{\lambda\sigma\}}{}^\kappa$, required in (151), since $\Gamma_{\nu\kappa}{}^\sigma = \Gamma_{\kappa\nu}{}^\sigma$, i.e the u^μ-space has no torsion. Inserting the equations (153) into the right-hand side of (151) we find the post-point expansion

$$\frac{i}{\hbar}\mathcal{A}_J^\epsilon = -\left[2\frac{\mathbf{u}_n \Delta \mathbf{u}_n}{\mathbf{u}_n^2} - \frac{\Delta \mathbf{u}_n{}^2}{\mathbf{u}_n^2} + 2\left(\frac{\mathbf{u}\Delta\mathbf{u}_n}{\mathbf{u}_n^2}\right)^2 + \dots\right]. \tag{155}$$

The measure of integration in (71) contains additional factors r_b, r_n, r_a which require further treatment. We shall rewrite it as

$$\begin{aligned} &\frac{(r_b/r_a)^{2\lambda-1}}{2\pi i\epsilon_s\hbar} \prod_{n=1}^{N} \left[\int \frac{d^2\Delta x_n}{2\pi i \epsilon_s r_{n-1}/M}\right] \\ &\approx \frac{1}{2\pi i\epsilon_s\hbar} \prod_{n=1}^{N} \left[\int \frac{d^2\Delta x_n}{2\pi i\epsilon_s\hbar r_n/M}\right] \prod_{n=1}^{N+1} \left[\left(\frac{r_n}{r_{n-1}}\right)\right]^{2\lambda} \\ &= \frac{1}{2\pi i\epsilon_s\hbar} \prod_{n=2}^{N+1} \left[\int \frac{d^2\Delta x_n}{2\pi i\epsilon_s\hbar r_n/M}\right] \exp\left\{\frac{i}{\hbar}\mathcal{A}_f^N\right\}. \end{aligned} \tag{156}$$

On the left-hand side we have shifted the labels n by one unit making use of the fact that with $\Delta\mathbf{x}_n = \mathbf{x}_n - \mathbf{x}_{n-1}$ we can certainly write $\prod_{n=2}^{N+1} \int d^2\Delta x_n = \prod_{n=1}^{N} \int d^2\Delta x_n$. Then we have raised the factors $1/r_{n-1}$ in the integrals to $1/r_n$ by means of an extra product $\prod_{n=1}^{N+1}(r_n/r_{n-1})$ and distributed the prefactor $(r_b/r_a)^{2\lambda-1}$ evenly over all slices as $\prod_{n=1}^{N+1}(r_n/r_{n-1})^{2\lambda-1}$. This gives the right-hand side of (156). There is only an error of order ϵ_s^2, made at the upper end (indicated by the symbol $\approx$ rather than $=$), which can be ignored. In the last equation we have introduced an effective action due to the $(r_n/r_{n-1})^{2\lambda}$ factors, for each time slice,

$$\frac{i}{\hbar}\mathcal{A}_f^\epsilon = 2\lambda \log \frac{r_n^2}{r_{n-1}^2} = 2\lambda \log \frac{\mathbf{u}_n^2}{\mathbf{u}_{n-1}^2}, \tag{157}$$

and for the sum over all slices

$$\mathcal{A}_f^N \equiv \sum_{n=1}^{N+1} \mathcal{A}_f^\epsilon. \tag{158}$$

The subscript f indicates that the general origin of this term are the rescaling factors $f_l(\mathbf{x}_b), f_r(\mathbf{x}_a)$.

We now go over from the $\Delta\mathbf{x}_n$ to the $\Delta\mathbf{u}_n$ integrations using the relation

$$d^2\Delta x = d^2\Delta u \;\; \exp\left\{\frac{i}{\hbar}\mathcal{A}_J^\epsilon\right\}, \tag{159}$$

and the measure becomes

$$\frac{1}{2}\frac{4}{2\cdot 2\pi i\epsilon_s\hbar}\prod_{n=1}^{N}\left(\frac{4d^2\Delta u_n}{2\cdot 2\pi i\epsilon_s\hbar/M}\right)\exp\left\{\frac{i}{\hbar}(\mathcal{A}_J^N+\mathcal{A}_f^N)\right\}, \tag{160}$$

where $\mathcal{A}_J^N$ is the sum over all time sliced Jacobian action pieces $\mathcal{A}_J^\epsilon$ of (155),

$$\mathcal{A}_J^N \equiv \sum_{n=1}^{N+1}\mathcal{A}_J^\epsilon. \tag{161}$$

The extra factors 2 in the denominators of (160) account for the fact that we want to integrate $\mathbf{u}_n$ over the entire u^μ-space. Then the x^i-space is traversed twice and we have to correct for this.

The time-sliced expression (160) has an important feature which was absent in the continuous formulation. It possesses dominant contributions not only for $\mathbf{u}_n \sim \mathbf{u}_{n-1}$, in which case $(\Delta\mathbf{u}_n)^2$ is of order ϵ_s, but also for $\mathbf{u}_n \sim -\mathbf{u}_{n-1}$ with $(\bar{\mathbf{u}}_n)^2$ of order ϵ_s. This is understandable since both situations correspond to $\mathbf{x}_n$ close to $\mathbf{x}_{n-1}$. The two cases have to be treated separately. Fortunately, by symmetry, both give the same contributions so that we need to treat only the case $\mathbf{u}_n \sim \mathbf{u}_{n-1}$ and drop the factors 2 in the denominators of the measure.

Before proceeding we expand the action $\mathcal{A}_f^\epsilon$ in the measure (160) around the post-point and find

$$\begin{aligned}\frac{i}{\hbar}\mathcal{A}_f^\epsilon &= 2\lambda\log\left(\frac{\mathbf{u}_n^2}{\mathbf{u}_{n-1}^2}\right)\\ &= 2\lambda\left[2\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2}-\frac{\Delta\mathbf{u}_n{}^2}{\mathbf{u}_n^2}+2\left(\frac{\mathbf{u}\Delta\mathbf{u}_n}{\mathbf{u}_n^2}\right)^2+\ldots\right].\end{aligned} \tag{162}$$

Comparison with (155) shows that when adding $(i/\hbar)\mathcal{A}_f^\epsilon$ and $(i/\hbar)\mathcal{A}_J^\epsilon$ this merely changes 2λ in $\mathcal{A}_f^\epsilon$ into $2\lambda - 1$.

Thus, altogether, the time-slicing produces the following short-time action

$$\mathcal{A}^{\epsilon} = \mathcal{A}_0^{\epsilon} + \Delta_{tot}\mathcal{A}^{\epsilon}, \tag{163}$$

with the leading free particle action

$$\mathcal{A}_0^{\epsilon}(\Delta\mathbf{u}_n) = 4M\frac{(\Delta\mathbf{u}_n)^2}{2\epsilon_s}, \tag{164}$$

plus the total correction term

$$\begin{aligned}
\frac{i}{\hbar}\Delta_{tot}\mathcal{A}^{\epsilon} &\equiv \frac{i}{\hbar}(\Delta\mathcal{A}^{\epsilon} + \mathcal{A}_J^{\epsilon} + \mathcal{A}_f^{\epsilon}) \\
&= \frac{i}{\hbar}4M\frac{\Delta\mathbf{u}_n{}^2}{2\epsilon_s}\left[(2\lambda-1)\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2} + \left(\frac{1}{4}-\lambda\right)\frac{\Delta\mathbf{u}_n{}^2}{\mathbf{u}_n^2} + 2\lambda^2\left(\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2}\right)^2\right] \\
&\quad +(2\lambda-1)\left[2\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2} - \frac{\Delta\mathbf{u}_n{}^2}{\mathbf{u}_n^2} + 2\left(\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2}\right)^2\right] + \dots\ .
\end{aligned} \tag{165}$$

We now show that the action $\Delta_{tot}\mathcal{A}^{\epsilon}$ is equivalent to zero in the sense that the kernel associated with the short-time action,

$$K^{\epsilon}(\Delta\mathbf{u}) = \frac{4}{2\cdot 2\pi i\epsilon_s\hbar/M}\exp\left\{\frac{i}{\hbar}(\mathcal{A}_0^{\epsilon} + \Delta_{tot}\mathcal{A}^{\epsilon})\right\}, \tag{166}$$

is equivalent to the zeroth-order free-particle kernel

$$K_0^{\epsilon}(\Delta\mathbf{u}) = \frac{4}{2\cdot 2\pi i\epsilon_s\hbar/M}\exp\left\{\frac{i}{\hbar}\mathcal{A}_0^{\epsilon}\right\}. \tag{167}$$

The equivalence is established by checking the moment conditions [see Ref. [2], Eqs. (11.48) - (11.50)]. For the kernel (166) we identify the correction factor

$$C_1 = C = \exp\left\{\frac{i}{\hbar}\Delta_{tot}\mathcal{A}^{\epsilon}\right\} - 1, \tag{168}$$

to be compared with the trivial factor C of the kernel (167),

$$C_2 = 0. \tag{169}$$

Hence, to prove equivalence we simply must show that

$$\begin{aligned} \langle C\rangle_0 &= 0, \\ \langle C\ (\mathbf{p}\Delta\mathbf{u})\rangle_0 &= 0 \end{aligned} \tag{170}$$

(omitting again the subscripts n).

The basic correlation functions due to $K_0^\epsilon(\Delta\mathbf{u})$ are

$$\langle \Delta u^\mu \Delta u^\nu \rangle_0 \equiv \frac{i\hbar\epsilon_s}{4M}\delta^{\mu\nu}. \tag{171}$$

We also need the higher correlations

$$\langle \Delta u^{\mu_1} \dots \Delta u^{\mu_{2n}} \rangle_0 = \left(\frac{i\hbar\epsilon_s}{4M}\right)^n \delta^{\mu_1 \dots \mu_{2n}}, \tag{172}$$

where the tensors $\delta^{\mu_1 \dots \mu_{2n}}$ are determined recursively, as in (8.62), by

$$\delta^{\mu_1 \dots \mu_{2n}} \equiv \delta^{\mu_1\mu_2}\delta^{\mu_3\mu_4 \dots \mu_{2n}} + \delta^{\mu_1\mu_3}\delta^{\mu_2\mu_4 \dots \mu_{2n}} + \dots + \delta^{\mu_1\mu_{2n}}\delta^{\mu_2\mu_3 \dots \mu_{2n-1}}. \tag{173}$$

They consists of $(2n-1)!!$ products of pair contractions $\delta^{\mu_i\mu_j}$. More specifically, in calculating (170) we encounter expectations of the following type

$$\langle (\Delta\mathbf{u})^{2k} (\mathbf{u}\Delta\mathbf{u})^{2l} \rangle_0 = \left(\frac{i\hbar\epsilon_s}{4M}\right)^{k+l} \frac{[D+2(k+l-1)]!!}{(D+2l-2)!!} (2l-1)!!(\mathbf{u}^2)^l, \tag{174}$$

and

$$\langle (\Delta\mathbf{u})^{2k} (\mathbf{u}\Delta\mathbf{u})^{2l} (\mathbf{u}\Delta\mathbf{u})(\mathbf{p}\Delta\mathbf{u}) \rangle_0 = \left(\frac{i\hbar\epsilon_s}{4M}\right)^{k+l+1} \frac{[D+2(k+l)]!!}{(D+2l)!!} (2l-1)!!\mathbf{u}\mathbf{p}, \tag{175}$$

where we have allowed for a general dimension D of the $\mathbf{u}$-space. Expanding (170) we now check that, for all terms of order ϵ_s,

$$\langle C\rangle_0 = \frac{i}{\hbar}\langle \Delta_{tot}\mathcal{A}^\epsilon\rangle_0 + \frac{1}{2!}\left(\frac{i}{\hbar}\right)^2 \langle (\Delta_{tot}\mathcal{A}^\epsilon)^2\rangle_0 = 0, \tag{176}$$

and

$$\langle C\ (\mathbf{p}\Delta\mathbf{u})\rangle_0 = \frac{i}{\hbar}\langle \Delta_{tot}\mathcal{A}^\epsilon\ (\mathbf{p}\Delta\mathbf{u})\rangle_0 = 0. \tag{177}$$

Indeed, the first term in (176) gives

$$\frac{i}{\hbar}\langle \Delta_{tot}\mathcal{A}^{\epsilon}\rangle_0 = 2i\frac{\hbar\epsilon_s}{M}\left\{-\left(\frac{1}{4}-\lambda\right)\frac{(D+2)D}{16} - 2\lambda^2\frac{D+2}{16}\right\}, \tag{178}$$

i.e., for $D = 2$,

$$\frac{i}{\hbar}\langle \Delta_{tot}\mathcal{A}^{\epsilon}\rangle_0 = -i\frac{\hbar\epsilon_s}{M}\left(\lambda - \frac{1}{2}\right)^2. \tag{179}$$

The second term cancels this identically in λ, being

$$\begin{aligned}\frac{1}{2!}\left(\frac{i}{\hbar}\right)^2\langle(\Delta_{tot}\mathcal{A}^{\epsilon})^2\rangle_0 &= \frac{1}{2}i\frac{\hbar\epsilon_s}{M} \qquad (180)\\ &\times\left\{4(2\lambda-1)^2\frac{(D+4)(D+2)}{64} + 4(2\lambda-1)^2\frac{1}{4} - 8(2\lambda-1)^2\frac{D+2}{16}\right\},\end{aligned}$$

i.e., for $D = 2$,

$$\frac{1}{2!}\left(\frac{i}{\hbar}\right)^2\langle(\Delta_{tot}\mathcal{A}^{\epsilon})^2\rangle_0 = i\frac{\hbar\epsilon_s}{M}\left(\lambda - \frac{1}{2}\right)^2. \tag{181}$$

But also the expectation (177),

$$\langle \Delta_{tot}\mathcal{A}^{\epsilon}\,(\mathbf{p}\Delta\mathbf{u})\rangle_0 = -\frac{\hbar^2\epsilon_s}{4M}[(2\lambda-1)(D+2)/4 - (2\lambda-1)], \tag{182}$$

vanishes identically in λ for $D = 2$.

Thus there is no finite time-slicing correction to the naive transformation of the H atom path integral in $D = 2$ dimensions so that it reduces indeed to the pure harmonic oscillator path integral given above.

4.4.3 D=3

Let us now prove the same thing for the case $D = 3$. As in Eq. (165), the action $\mathcal{A}_E^N$ in the time-sliced path integral has to be supplemented, in each slice, by the Jacobian action

$$\begin{aligned}\frac{i}{\hbar}\mathcal{A}_J^{\epsilon} &= -e^{\mu}{e^i}_{\{\mu,\nu\}}\Delta u^{\nu} - {e_i}^{\mu}{e^i}_{\{\kappa,\nu\}}{e_j}^{\kappa}{e^i}_{\{\mu,\lambda\}}\Delta u^{\nu}\Delta u^{\lambda}\\ &= -{\Gamma_{\{\nu\mu\}}}^{\mu}\Delta u^{\nu} - \frac{1}{2}{\Gamma_{\{\nu\kappa\}}}^{\sigma}{\Gamma_{\{\lambda\sigma\}}}^{\kappa}\Delta u^{\nu}\Delta u^{\lambda}.\end{aligned} \tag{183}$$

The basis tetrad

$$e^i{}_\mu = \partial x^i/\partial u^\mu = 2A^i{}_\mu(\vec{u}) \tag{184}$$

is now given by the 4×4 matrix (15), with the reciprocal tetrad,

$$e_i{}^\mu = \frac{1}{2\vec{u}^2} e^i{}_\mu. \tag{185}$$

From this we find the matrix components of the connection,

$$\begin{aligned}
(\Gamma_1)_\mu{}^\nu &= \frac{1}{\vec{u}^2}\begin{pmatrix} u^1 & u^2 & -u^3 & -u^4 \\ -u^2 & u^1 & -u^4 & u^3 \\ u^3 & u^4 & u^1 & u^2 \\ u^4 & -u^3 & -u^2 & u^1 \end{pmatrix}_\mu{}^\nu, \\
(\Gamma_2)_\mu{}^\nu &= \frac{1}{\vec{u}^2}\begin{pmatrix} u^2 & -u^1 & u^4 & -u^3 \\ u^1 & u^2 & -u^3 & -u^4 \\ -u^4 & u^3 & u^2 & -u^1 \\ u^3 & u^4 & u^1 & u^2 \end{pmatrix}_\mu{}^\nu, \\
(\Gamma_3)_\mu{}^\nu &= \frac{1}{\vec{u}^2}\begin{pmatrix} u^3 & u^4 & u^1 & u^2 \\ -u^4 & u^3 & u^2 & -u^1 \\ -u^1 & -u^2 & u^3 & u^4 \\ -u^2 & u^1 & -u^4 & u^3 \end{pmatrix}_\mu{}^\nu, \\
(\Gamma_4)_\mu{}^\nu &= \frac{1}{\vec{u}^2}\begin{pmatrix} u^4 & -u^3 & -u^2 & u^1 \\ u^3 & u^4 & u^1 & u^2 \\ u^2 & -u^1 & u^4 & -u^3 \\ -u^1 & -u^2 & u^3 & u^4 \end{pmatrix}_\mu{}^\nu.
\end{aligned} \tag{186}$$

As in the two-dimensional case, the connection satisfies an important identity

$$\Gamma_\mu{}^{\mu\nu} \equiv 0, \tag{187}$$

which is really the essential reason for the absence of the time slicing corrections to be proved in this section. As in two dimensions, (187) this is a consequence of the identity

$$\partial_\mu e^i{}_\mu \equiv 0. \tag{188}$$

There is now, however, an important difference with respect to the two-dimensional case. The present mapping $dx^i = e^i{}_\mu(u)du^\mu$ is not integrable.

As a consequence, the u^μ-space carries a torsion $S_{\mu\nu}{}^\lambda$ with the nonzero components

$$S_{12}{}^\lambda = S_{34}{}^\lambda = \frac{1}{\vec{u}^2}(-u^2, u^1, -u^4, u^3)^\lambda. \tag{189}$$

The once contracted torsion is

$$S_\mu = S_{\mu\nu}{}^\nu = \frac{u^\mu}{\vec{u}^2}. \tag{190}$$

For this reason, the contracted connections

$$\begin{aligned} \Gamma_{\nu\mu}{}^\mu &= e_i{}^\mu \partial_\nu e^i{}_\mu = \frac{4u^\nu}{\vec{u}^2}, \\ \Gamma_{\mu\nu}{}^\mu &= -e^i{}_\nu \partial_\mu e_i{}^\mu = \frac{2u^\nu}{\vec{u}^2}, \end{aligned} \tag{191}$$

are no longer equal, as they were in (153). Symmetrization in the lower indices gives

$$\Gamma_{\{\nu\mu\}}{}^\mu = \frac{3u^\nu}{\vec{u}^2}. \tag{192}$$

Due to this, the $\Delta u^\nu \Delta u^\lambda$ terms in (151) are, in contrast to the two-dimensional expressions, not given directly by

$$\Gamma_{\nu\kappa}{}^\sigma \Gamma_{\lambda\sigma}{}^\kappa = -\frac{4}{\vec{u}^4}(\delta^{\nu\lambda}\vec{u}^2 - 2u^\nu u^\lambda), \tag{193}$$

but due to the nonzero torsion we must symmetrize the lower indices,

$$\begin{aligned} \Gamma_{\{\nu\kappa\}}{}^\sigma \Gamma_{\{\lambda\sigma\}}{}^\kappa &= \Gamma_{\nu\kappa}{}^\sigma \Gamma_{\lambda\sigma}{}^\kappa - 2\Gamma_{\nu\kappa}{}^\sigma S_{\lambda\sigma}{}^\kappa + S_{\nu\kappa}{}^\sigma S_{\lambda\sigma}{}^\kappa \\ &= \Gamma_{\nu\kappa}{}^\sigma \Gamma_{\lambda\sigma}{}^\kappa - 2(-\delta_{\nu\lambda}\vec{u}^2 + 2u_\nu u_\lambda)/\vec{u}^4 + u_\nu u_\lambda/\vec{u}^4. \end{aligned} \tag{194}$$

Collecting these terms, the Jacobian action (183) becomes

$$\frac{i}{\hbar}\mathcal{A}_J^\epsilon = -\left[3\frac{\vec{u}_n \Delta\vec{u}_n}{\vec{u}_n^2} - \frac{\Delta\vec{u}_n{}^2}{\vec{u}_n^2} + \frac{5}{2}\left(\frac{\vec{u}_n\Delta\vec{u}_n}{\vec{u}_n^2}\right)^2 + \dots\right]. \tag{195}$$

In contrast to the two-dimensional case [see (155)], this cannot be incorporated into $\mathcal{A}_f^\epsilon$, which is now [see (117)]

$$\begin{aligned} \frac{i}{\hbar}\mathcal{A}_f^\epsilon &= 3\lambda \log\left(\frac{\vec{u}_n^2}{\vec{u}_{n-1}^2}\right) \\ &= 3\lambda \log\left[2\frac{\vec{u}_n\Delta\vec{u}_n}{\vec{u}_n^2} - \frac{\Delta\vec{u}_n{}^2}{\vec{u}_n^2} + 2\left(\frac{\vec{u}\Delta\vec{u}_n}{\vec{u}_n^2}\right)^2 + \dots\right]. \end{aligned} \tag{196}$$

We may, however, write (omitting the subscripts n)

$$\frac{i}{\hbar}\mathcal{A}_J^\epsilon = -2\log\left(\frac{\vec{u}^2}{(\vec{u}-\Delta\vec{u})^2}\right) + \frac{\vec{u}\Delta\vec{u}}{\vec{u}^2} - \frac{\Delta\vec{u}^2}{\vec{u}^2} + \frac{3}{2}\left(\frac{\vec{u}\Delta\vec{u}}{\vec{u}^2}\right)^2 + \dots, \tag{197}$$

and absorb the first term into $\mathcal{A}_f^\epsilon$ by changing 3λ to $(3\lambda-2)$. Thus, we obtain altogether the additional action [to be compared with (165)]

$$\begin{aligned}\frac{i}{\hbar}\Delta_{tot}\mathcal{A}^\epsilon &= \frac{i}{\hbar}4M\frac{\Delta\vec{u}^2}{2\epsilon}\left[(2\lambda-1)\frac{\vec{u}\Delta\vec{u}}{\vec{u}^2} + (\frac{1}{4}-\lambda)\frac{\Delta\vec{u}^2}{\vec{u}^2} + 2\lambda^2\left(\frac{\vec{u}\Delta\vec{u}}{\vec{u}^2}\right)^2\right] \\ &\quad +(3\lambda-2)\left[2\frac{\vec{u}\Delta\vec{u}}{\vec{u}^2} - \frac{\Delta\vec{u}^2}{\vec{u}^2} + 2\left(\frac{\vec{u}\Delta\vec{u}}{\vec{u}^2}\right)^2\right] \\ &\quad +\frac{\vec{u}\Delta\vec{u}}{\vec{u}^2} - \frac{(\Delta\vec{u})^2}{\vec{u}^2} + \frac{3}{2}\left(\frac{\vec{u}\Delta\vec{u}}{\vec{u}^2}\right)^2 + \dots .\end{aligned} \tag{198}$$

We are now able to show that the expansion of the correction

$$C = \exp\left\{\frac{i}{\hbar}\Delta_{tot}\mathcal{A}^\epsilon\right\} - 1 \tag{199}$$

has the vanishing expectations,

$$\begin{aligned}\langle C\rangle_0 &= 0, \\ \langle C\ (\vec{p}\Delta\vec{u})\rangle_0 &= 0,\end{aligned} \tag{200}$$

i.e.,

$$\frac{i}{\hbar}\langle\Delta_{tot}\mathcal{A}^\epsilon\rangle_0 + \frac{1}{2}\left(\frac{i}{\hbar}\right)^2\langle(\Delta_{tot}\mathcal{A}^\epsilon)^2\rangle_0 = 0, \tag{201}$$

$$\frac{i}{\hbar}\langle\Delta_{tot}\mathcal{A}\ (\vec{p}\Delta\vec{u})\rangle_0 = 0, \tag{202}$$

as in (176), (177). In fact, using formula (175) the expectation (202) is immediately found to vanish identically in λ for $D=4$, being proportional to

$$i\left\{-2(2\lambda-1)\frac{D+2}{16} + 2(3\lambda-2)\frac{1}{4} + \frac{1}{4}\right\}. \tag{203}$$

Similarly, using formula (174), the first term in (201) has an expectation proportional to

$$i\left\{-2\left(\frac{1}{4}-\lambda\right)\frac{(D+2)D}{16}-4\lambda^2\frac{D+2}{16}-(3\lambda-2)\left(\frac{D}{4}-\frac{2}{4}\right)-\left(\frac{D}{4}-\frac{3}{8}\right)\right\}, \tag{204}$$

i.e., for $D=4$,

$$i\left\{-3\left(\frac{1}{4}-\lambda\right)-\frac{3}{2}\lambda^2-\frac{1}{2}(3\lambda-2)-\frac{5}{8}\right\}, \tag{205}$$

to which the second term adds

$$i\,\frac{1}{2}\left\{4(2\lambda-1)^2\frac{(D+4)(D+2)}{64}+9(2\lambda-1)^2\frac{1}{4}-12(2\lambda-1)^2\frac{D+2}{16}\right\}, \tag{206}$$

i.e., for $D=4$,

$$i\left\{\frac{3}{2}(2\lambda-1)^2+\frac{9}{8}(2\lambda-1)^2-\frac{9}{4}(2\lambda-1)^2\right\}. \tag{207}$$

Thus, just as in the two-dimensional case, the sum of all time slicing corrections vanishes. This completes the proof.

4.5 Brief Argument for Absence of Time Slicing Corrections

It was shown in the textbook [2] that the basic reason for the absence of the time slicing corrections is the property of the connection

$$\Gamma_\mu{}^{\mu\lambda}=g^{\mu\nu}e_i{}^\lambda\partial_\mu e^i{}_\nu=0, \tag{208}$$

which follows from the property of the basis tetrad, $\partial_\mu e^i_\mu=0$, together with the diagonality of $g^{\mu\nu}\propto\delta_{\mu\nu}$. The reader is referred to Section 13.6 of [2] for details. It is thanks to this fortunate circumstance $\Gamma_\mu{}^{\mu\lambda}=0$ that the formal solution found by Duru and Kleinert in 1979 happened to be ultimately correct.

For the same reason, the path integral of the dionium system consisting of an electric and a magnetic point charge can be integrated without time-slicing corrections. See Section 14.6 of [2].

5 Summary

The H atom, as simple as it is, has revealed many interesting algebraic and path integral features. Both have led to new tyes of solutions of many other quantum mechanical systems.

A particularly interesting feature which has come up only in the recent development is that the transformation which makes the path integral solution possible by carrying the system into a harmonic oscillator transforms a flat space into one with curvature and torsion. Thus, as a mathematical artifact, the H atom provides us a system on which we can test whether our quantum mechanical principles work correctly in general metric-affine spaces. In this role it has rendered us a significant test for the correctness of a recently proposed quantum equivalence principle which tells us how to take the path integral formalism from a flat space into a space with curvature and torsion [8, 2]. It may be the only such system for a long time to come since examples in gravitational physics are not expected to be available for many years.

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