Et modo quae fuerat semita, facta via est
What was only a path is now made a high road
Martial (40–103), Epig., Book 7, 60

13

Path Integral of Coulomb System

One of the most important successes of Schrödinger quantum mechanics is the explanation of the energy levels and transition amplitudes of the hydrogen atom. Within the path integral formulation of quantum mechanics, this fundamental system has resisted for many years all attempts at a solution. An essential advance was made in 1979 when Duru and Kleinert [1] recognized the need to work with a generalized pseudotime-sliced path integral of the type described in Chapter 12. After an appropriate coordinate transformation the path integral became harmonic and solvable. A generalization of this two-step transformation has meanwhile led to the solution of many other path integrals to be presented in Chapter 14. The final solution of the problem turned out to be quite subtle due to the nonholonomic nature of the subsequent coordinate transformation which required the development of a correct path integral in spaces with curvature and torsion [2], as done in Chapter 10. Only this made it possible to avoid unwanted fluctuation corrections in the Duru-Kleinert transformation of the Coulomb system, a problem in all earlier attempts.

The first consistent solution was presented in the first edition of this book in 1990.

13.1 Pseudotime Evolution Amplitude

Consider the path integral for the time evolution amplitude of an electron-proton system with a Coulomb interaction. If $m_{\rm e}$ and $m_{\rm p}$ denote the masses of the two particles whose reduced mass is $M = m_{\rm e}m_{\rm p}/(m_{\rm e}+m_{\rm p})$, and if e is the electron charge, the system is governed by the Hamiltonian

$$H = \frac{p^2}{2M} - \frac{e^2}{r}. \tag{13.1}$$

The formal continuum path integral for the time evolution amplitude reads

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a) = \int \mathcal{D}^3x(t) \exp\left[\frac{i}{\hbar}\int_{t_b}^{t_a} dt(\mathbf{p}\dot{\mathbf{x}} - H)\right]. \tag{13.2}$$

As observed in the last chapter, its Euclidean version cannot be time-sliced into a finite number of integrals since the paths would collapse. The paths would stretch out into a straight line with $\dot{\mathbf{x}} \approx 0$ and slide down into the $1/r$-abyss. A path integral whose Euclidean version is stable can be written down using the pseudotime evolution amplitude (12.28). A convenient family of regulating functions is

$$f_l(\mathbf{x}) = f(\mathbf{x})^{1-\lambda}, \quad f_r(\mathbf{x}) = f(\mathbf{x})^{\lambda}, \tag{13.3}$$

whose product satisfies $f_l(\mathbf{x})f_r(\mathbf{x}) = f(\mathbf{x}) = r$. Since the path integral represents the general resolvent operator (12.21), all results must be independent of the splitting parameter λ after going to the continuum limit. This independence is useful in checking the calculations.

Thus we consider the fixed-energy amplitude

$$(\mathbf{x}_b|\mathbf{x}_a)_E = \int_0^\infty dS \langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle, \tag{13.4}$$

with the pseudotime-evolution amplitude

$$\langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle = r_b^\lambda\, r_a^{1-\lambda} \int \mathcal{D}^D x(s) \int \frac{\mathcal{D}^D p(s)}{(2\pi\hbar)^D} \exp\left\{\frac{i}{\hbar}\int_0^S ds[\mathbf{p}\mathbf{x}' - r^{1-\lambda}(H-E)r^\lambda]\right\}, \tag{13.5}$$

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. After time slicing and with the notation $\Delta\mathbf{x}_n \equiv \mathbf{x}_n - \mathbf{x}_{n-1}$, $\epsilon_s \equiv S/(N+1)$, the amplitude (13.5) reads

$$\langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle \approx r_b^\lambda r_a^{1-\lambda} \prod_{n=2}^{N+1}\left[\int_{-\infty}^{\infty} d^D\Delta x_n\right] \prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{d^D p_n}{(2\pi\hbar)^D}\right] e^{i\mathcal{A}_E^N/\hbar}, \tag{13.6}$$

where the action is

$$\mathcal{A}_E^N[\mathbf{p},\mathbf{x}] = \sum_{n=1}^{N+1}\left[\mathbf{p}_n\,\Delta\mathbf{x}_n - \epsilon_s\, r_n^{1-\lambda} r_{n-1}^\lambda\left(\frac{\mathbf{p}_n{}^2}{2M} - E\right) + \epsilon_s\, e^2\right]. \tag{13.7}$$

The term $\epsilon_s\, e^2$ carries initially a factor $(r_{n-1}/r_n)^\lambda$ which is dropped, since it is equal to unity in the continuum limit. When integrating out the momentum variables, $N+1$ factors $1/(r_n^{1-\lambda}\, r_{n-1}^\lambda)^{D/2}$ appear. After rearranging these, the configuration space path integral becomes

$$\langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle \approx \frac{r_b^\lambda r_a^{1-\lambda}}{\sqrt{2\pi\, i\epsilon_s\hbar\, r_b^{1-\lambda}\, r_a^\lambda/M}^D} \prod_{n=2}^{N+1}\left[\int \frac{d^D\Delta\mathbf{x}_n}{\sqrt{2\pi i\epsilon_s\hbar r_{n-1}/M}^D}\right] e^{i\mathcal{A}_E^N[\mathbf{x},\mathbf{x}']/\hbar}, \tag{13.8}$$

with the pseudotime-sliced action

$$\mathcal{A}_E^N[\mathbf{x},\mathbf{x}'] = (N+1)\epsilon_s e^2 + \sum_{n=1}^{N+1}\left[\frac{M}{2}\frac{(\Delta\mathbf{x}_n)^2}{\epsilon_s r_n^{1-\lambda}\, r_{n-1}^\lambda} + \epsilon_s\, r_n E\right]. \tag{13.9}$$

In the last term, we have replaced $r_n^{1-\lambda} r_{n-1}^{\lambda}$ by r_n without changing the continuum limit. The limiting action can formally be written as

$$\mathcal{A}_E[\mathbf{x}, \mathbf{x}'] = e^2 S + \int_0^S ds \left(\frac{M}{2r} \mathbf{x}'^2 + Er \right). \tag{13.10}$$

We now solve the Coulomb path integral first in two dimensions, assuming that the movement of the electron is restricted to a plane while the electric field extends into the third dimension. Afterwards we proceed to the physical three-dimensional system. The case of an arbitrary dimension D will be solved in Chapter 14. The one-dimensional case will not be treated here. The exact energy levels were found before at the and of Section 4.1 from a semiclassical expansion. For a long time, the one-dimensional Coulomb system was only of mathematical interest. Recently, however, it has received increased attention due to the possibility of forming hydrogen-like bound states in *quantum wires* [3].

13.2 Solution for the Two-Dimensional Coulomb System

First we observe that the kinetic pseudoenergy has a scale dimension $[rp^2] \sim [r^{-1}]$ which is precisely opposite to that of the potential term $[r^{+1}]$. The dimensional situation is similar to that of the harmonic oscillator, where the dimensions are $[p^2] = [r^{-2}]$ and $[r^{+2}]$, respectively. It is possible make the correspondence perfect by describing the Coulomb system in terms of "square root coordinates", i.e., by transforming $r \to u^2$. In two dimensions, the appropriate square root is given by the *Levi-Civita transformation*

$$\begin{aligned} x^1 &= (u^1)^2 - (u^2)^2, \\ x^2 &= 2u^1 u^2. \end{aligned} \tag{13.11}$$

If we imagine the vectors $\mathbf{x}$ and $\mathbf{u}$ to move in the complex planes parametrized by $x = x^1 + ix^2$ and $u = u^1 + iu^2$, the transformed variable u corresponds to the complex square root:

$$u = \sqrt{x}. \tag{13.12}$$

Let us also introduce the matrix

$$A(\mathbf{u}) = \begin{pmatrix} u^1 & -u^2 \\ u^2 & u^1 \end{pmatrix}, \tag{13.13}$$

and write (13.11) as a matrix equation:

$$\mathbf{x} = A(\mathbf{u})\mathbf{u}. \tag{13.14}$$

The Levi-Civita transformation is an integrable coordinate transformation which carries the flat x^i-space into a flat u^μ-space. We mention this fact since in the later treatment of the three-dimensional hydrogen atom, the transition to the "square root coordinates" will require a nonintegrable (nonholonomic) coordinate transformation defined only differentially. As explained in Chapter 10, such mappings change, in general, a flat Euclidean space into a space with curvature and torsion. The generation of torsion is precisely the reason why the three-dimensional system remained unsolved until 1990. In two dimensions, this phenomenon happens to be absent.

If we write the transformation (13.11) in terms of a basis dyad $e^i_\mu(\mathbf{u})$ as $dx^i = e^i{}_\mu(\mathbf{u})\, du^\mu$, this is given by

$$e^i{}_\mu(\mathbf{u}) = \frac{\partial x^i}{\partial u^\mu}(\mathbf{u}) = 2A^i{}_\mu(\mathbf{u}), \tag{13.15}$$

with the reciprocal dyad

$$e_i{}^\mu(\mathbf{u}) = \frac{1}{2}(A^{-1})^T{}_i{}^\mu(\mathbf{u}) = \frac{1}{2\mathbf{u}^2} A^i{}_\mu(\mathbf{u}). \tag{13.16}$$

The associated affine connection

$$\Gamma_{\mu\nu}{}^\lambda = e_i{}^\lambda\, \partial_\mu\, e^i{}_\nu = \frac{1}{\mathbf{u}^2}[(\partial_\mu A)^T A]_{\nu\lambda} \tag{13.17}$$

has the matrix elements $(\Gamma_\mu)_\nu{}^\lambda = \Gamma_{\mu\nu}{}^\lambda$:

$$\begin{aligned}
(\Gamma_1)_\mu{}^\nu &= \frac{1}{\mathbf{u}^2}\begin{pmatrix} u^1 & -u^2 \\ u^2 & u^1 \end{pmatrix}_\mu{}^\nu = \frac{1}{2\mathbf{u}^2}\, A(\mathbf{u})^\mu{}_\nu, \\
(\Gamma_2)_\mu{}^\nu &= \frac{1}{\mathbf{u}^2}\begin{pmatrix} u^2 & u^1 \\ -u^1 & u^2 \end{pmatrix}_\mu{}^\nu .
\end{aligned} \tag{13.18}$$

The affine connection satisfies the important identity

$$\Gamma_\mu{}^{\mu\lambda} \equiv 0, \tag{13.19}$$

which follows from the defining relation

$$\Gamma_\mu{}^{\mu\lambda} \equiv g^{\mu\nu} e_i{}^\lambda\, \partial_\mu\, e^i{}_\nu, \tag{13.20}$$

by inserting the obvious special property of $e^i{}_\mu$

$$\partial_\mu e^i{}_\mu = \partial^2_{\mathbf{u}}\, x^i(\mathbf{u}) = 0, \tag{13.21}$$

using the diagonality of $g^{\mu\nu} = \delta^{\mu\nu}/4r$.

The identity (13.19) will be shown in Section 13.6 to be the essential geometric reason for the absence of the time slicing corrections.

The torsion and the Riemann-Cartan curvature tensor vanish identically, the former because of the specific form of the matrix elements (13.18), the latter due to the linearity of the basis dyads $e^i{}_\mu(\mathbf{u})$ in $\mathbf{u}$ which guarantees trivially the integrability conditions, i.e.,

$$\begin{aligned}
e_i{}^\lambda\, (\partial_\mu\, e^i{}_\nu - \partial_\nu\, e^i{}_\mu) &\equiv 0, & (13.22)\\
e_i{}^\kappa (\partial_\mu\, \partial_\nu - \partial_\nu\, \partial_\mu)\, e^i{}_\lambda &\equiv 0, & (13.23)
\end{aligned}$$

and thus $S_{\mu\nu}{}^{\lambda} \equiv 0$, $R_{\mu\nu\lambda}{}^{\kappa} \equiv 0$.

In the continuum limit, the Levi-Civita transformation converts the action (13.10) into that of a harmonic oscillator. With

$$\mathbf{x}'^2 = 4\mathbf{u}^2\,\mathbf{u}'^2 = 4r\,\mathbf{u}'^2 \tag{13.24}$$

we find

$$\mathcal{A}[\mathbf{x}] = e^2 S + \int_0^S ds\left(\frac{4M}{2}\mathbf{u}'^2 + E\mathbf{u}^2\right). \tag{13.25}$$

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

$$\mathcal{A}_{\rm os}[\mathbf{u}] = \int_0^S ds\frac{\mu}{2}(\mathbf{u}'^2 - \omega^2\mathbf{u}^2), \tag{13.26}$$

which oscillates in the pseudotime s with an effective mass

$$\mu = 4M, \tag{13.27}$$

and a pseudofrequency

$$\omega = \sqrt{-E/2M}. \tag{13.28}$$

Note that ω has the dimension $1/s$ corresponding to $[\omega] = [r/t]$ (in contrast to a usual frequency whose dimension is $[1/t]$).

The path integral is well defined only as long as the energy E of the Coulomb system 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, the pseudotime-sliced amplitude is calculated as follows. Choosing a splitting parameter $\lambda = 1/2$ and ignoring for the moment all complications due to the finite time slicing, we deduce from (13.14) that

$$d\mathbf{x} = 2A(\mathbf{u})d\mathbf{u}, \tag{13.29}$$

and hence

$$d^2x_n = 4\mathbf{u}_n{}^2 d^2u_n. \tag{13.30}$$

Since the $\mathbf{x}$- and the $\mathbf{u}$-space are both Euclidean, the integrals over $\Delta\mathbf{x}_n$ in (13.8) can be rewritten as integrals over $\mathbf{x}_n$, and transformed directly to $\mathbf{u}_n$ variables. The result is

$$\langle\mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle = \frac{1}{4}e^{ie^2S/\hbar}[(\mathbf{u}_bS|\mathbf{u}_a0) + (-\mathbf{u}_bS|\mathbf{u}_a0)], \tag{13.31}$$

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

$$(\mathbf{u}_bS|\mathbf{u}_a0) \approx \frac{1}{2\pi i\hbar\epsilon_s/\mu}\prod_{n=1}^{N}\left[\int\frac{d^2u_n}{2\pi i\hbar\epsilon_s/\mu}\right] \times \exp\left\{\frac{i}{\hbar}\sum_{n=1}^{N}\frac{\mu}{2}\left(\frac{1}{\epsilon_s}\Delta\mathbf{u}_n{}^2 - \epsilon_s\omega^2\mathbf{u}_n{}^2\right)\right\}. \tag{13.32}$$

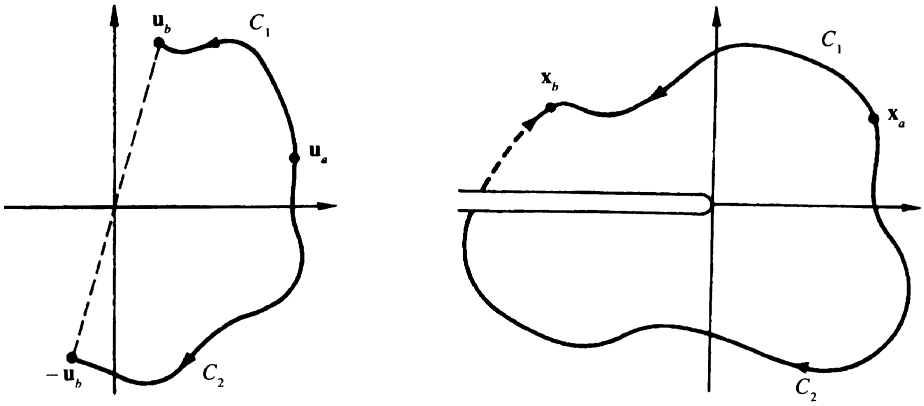

Figure 13.1 Illustration of associated final points in **u**-space, to be summed in the oscillator amplitude. In **x**-space, the paths run from $\mathbf{x}_a$ to $\mathbf{x}_b$ once directly and once after crossing the cut into the second sheet of the complex function $u = \sqrt{x}$.

The evaluation of the Gaussian integrals yields, in the continuum limit [recall (2.177)]:

$$(\mathbf{u}_b S|\mathbf{u}_a 0) = \frac{\mu\omega}{2\pi i\hbar \sin\omega S} \exp\left\{\frac{i}{2\hbar}\frac{\mu\omega}{\sin\omega S}[({\mathbf{u}_b}^2 + {\mathbf{u}_a}^2)\cos\omega S - 2\mathbf{u}_b\mathbf{u}_a]\right\}. \quad (13.33)$$

The symmetrization in $\mathbf{u}_b$ in Eq. (13.31) 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 $-\mathbf{u}_b$ (see Fig. 13.1).

The fixed-energy amplitude is obtained by the integral (13.4) over the pseudotime evolution amplitude (12.18):

$$(\mathbf{x}_b|\mathbf{x}_a)_E = \int_0^\infty dS\, e^{ie^2S/\hbar}\,\frac{1}{4}[(\mathbf{u}_b S|\mathbf{u}_a 0) + (-\mathbf{u}_b S|\mathbf{u}_a 0)]. \quad (13.34)$$

By inserting (13.33), this becomes

$$\begin{aligned}(\mathbf{x}_b|\mathbf{x}_a)_E &= \frac{1}{2}\int_0^\infty dS \exp(ie^2S/\hbar)F^2(S)\\ &\times \exp\left[-\pi F^2(S)(\mathbf{u}_b^2+\mathbf{u}_a^2)\cos\omega S\right]\,\cosh\left[2\pi F^2(S)\mathbf{u}_b\mathbf{u}_a\right], \quad (13.35)\end{aligned}$$

with the abbreviation

$$F(S) = \sqrt{\mu\omega/2\pi i\hbar\sin\omega S}, \quad (13.36)$$

for the one-dimensional fluctuation factor [recall (2.171)]. The coordinates $\mathbf{u}_b$ and $\mathbf{u}_a$ on the right-hand side are related to $\mathbf{x}_b\mathbf{x}_a$ on the left-hand side by

$$\mathbf{u}_{a,b}^2 = r_{a,b}, \quad \mathbf{u}_b\mathbf{u}_a = \sqrt{(r_br_a + \mathbf{x}_b\mathbf{x}_a)/2}. \quad (13.37)$$

When performing the integral over S, we have to pass around the singularities in $F(S)$ in accordance with the $i\eta$-prescription, replacing $\omega \to \omega - i\eta$. Equivalently, we can rotate the contour of S-integration to make it run along the negative imaginary semi-axis,

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

This amounts to going over to the Euclidean amplitude of the harmonic oscillator in which the singularities are completely avoided. The amplitude is rewritten in a more compact form by introducing the variables

$$\varrho \equiv e^{-2i\omega S} = e^{-2\omega\sigma}, \tag{13.38}$$

$$\kappa \equiv \frac{\mu\omega}{2\hbar} = \frac{2M\omega}{\hbar} = \sqrt{-2ME/\hbar^2}, \tag{13.39}$$

$$\nu \equiv \frac{e^2}{2\omega\hbar} = \sqrt{\frac{e^4 M}{-2\hbar^2 E}}. \tag{13.40}$$

Then

$$\pi F^2(S) = \kappa \frac{2\sqrt{\varrho}}{1-\varrho}, \tag{13.41}$$

$$e^{ie^2 s/\hbar} F^2(S) = \frac{2}{\pi}\kappa \frac{\varrho^{1/2-\nu}}{1-\varrho}, \tag{13.42}$$

and the fixed-energy amplitude of the two-dimensional Coulomb system takes the form

$$(\mathbf{x}_b|\mathbf{x}_a)_E = -i\frac{M}{\pi\hbar}\int_0^1 d\varrho\, \frac{\varrho^{-1/2-\nu}}{1-\varrho} \cos\left[2\kappa \frac{2\sqrt{\varrho}}{1-\varrho}\sqrt{(r_b r_a + \mathbf{x}_b \mathbf{x}_a)/2}\right] \times \exp\left[-\kappa \frac{1+\varrho}{1-\varrho}(r_b + r_a)\right]. \tag{13.43}$$

Note that the integral converges only for $\nu < 1/2$. Expanding the integrand in powers of ρ the integral can be done and yields a sum over terms $1/(\nu - 1/2), 1/(\nu - 3/2), \dots$. The residues can be factorized into a sum $e^{im\phi_b}e^{-im\phi_a} + e^{-im\phi_b}e^{im\phi_a}$, where ϕ are the azimuthal angle of the two-dimensional vectors $\mathbf{x}$. Thus we obtain a spectral decomposition of the amplitude:

$$(\mathbf{x}_b|\mathbf{x}_a)_E = \sum_{n=1}^{\infty} \frac{i\hbar}{E - E_n} \sum_{m=0}^{n-1} \left[\psi_{n_r,m}(\mathbf{x}_b)\psi^*_{n_r,m}(\mathbf{x}_b) + \psi_{n_r,-m}(\mathbf{x}_b)\psi^*_{n_r,-m}(\mathbf{x}_b)\right], \tag{13.44}$$

where

$$\psi_{n_r,m}(\mathbf{x}) = \frac{1}{\sqrt{r}} R_{n_r,|m|}(r) \frac{1}{\sqrt{2\pi}} e^{im\phi}, \quad r \equiv \tag{13.45}$$

are the wave functions and

$$E_n = -\frac{Me^4}{\hbar^4}\frac{1}{(n-\frac{1}{2})^2} \tag{13.46}$$

the energy eigenvalues. The *principal quantum number* n is related to the radial quantum number $n_r = 0, 1, 2, 3, \ldots$ and the azimuthal quantum number m by $n = n_r + |m| + 1$. The radial eigenfunctions are expressed in terms of confluent hypergeometric functions (9.45) as

$$\frac{1}{\sqrt{r}} R_{n_r,|m|}(r) = N_{n_r,|m|} \left(\frac{2r}{r_n}\right)^{|m|} e^{-r/r_n} {}_1F_1(-n + |m| + 1, 2|m| + 1, 2r/r_n), \quad (13.47)$$

where $r_n \equiv (n - \frac{1}{2})r_H = (n - 1/2)Me^2/\hbar^2$, and [5]

$$N_{n_r,|m|} \equiv \frac{2}{r_n} \frac{1}{2|m|!} \sqrt{\frac{(n + |m| - 1)!}{(2n - 1)(n - |m| - 1)!}}. \quad (13.48)$$

It is possible to write down another integral representation converging for all $\nu \neq 1/2,\, 3/2,\, 5/2, \ldots$. To do this we change the variable of integrations to

$$\zeta \equiv \frac{1 + \varrho}{1 - \varrho}, \quad (13.49)$$

so that

$$\frac{d\varrho}{(1 - \varrho)^2} = \frac{1}{2} d\zeta, \quad \varrho = \frac{\zeta - 1}{\zeta + 1}. \quad (13.50)$$

This leads to

$$(\mathbf{x}_b|\mathbf{x}_a)_E = -i\frac{M}{\pi\hbar} \frac{1}{2} \int_1^\infty d\zeta (\zeta - 1)^{-\nu-1/2} (\zeta + 1)^{\nu-1/2} \times \cos\left\{2\kappa\sqrt{\zeta^2 - 1}\sqrt{(r_b r_a + \mathbf{x}_b\mathbf{x}_a)/2}\right\} e^{-\kappa\zeta(r_b + r_a)}. \quad (13.51)$$

The integrand has a cut in the complex ζ-plane extending from $z = -1$ to $-\infty$ and from $\zeta = 1$ to ∞. The integral runs along the right-hand cut. The integral 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 may replace

$$\int_1^\infty d\zeta (\zeta - 1)^{-\nu-1/2} \ldots \to \frac{\pi e^{i\pi(\nu+1/2)}}{\sin[\pi(\nu + 1/2)]} \frac{1}{2\pi i} \int_C d\zeta (\zeta - 1)^{-\nu-1/2} \ldots\,, \quad (13.52)$$

and the fixed-energy amplitude reads

$$(\mathbf{x}_b|\mathbf{x}_a)_E = -i\frac{M}{\pi\hbar} \frac{1}{2} \frac{\pi e^{i\pi(\nu+1/2)}}{\sin[\pi(\nu + 1/2)]} \int_C \frac{d\zeta}{2\pi i} (\zeta - 1)^{-\nu-1/2} (\zeta + 1)^{\nu-1/2} \times \cos\left[2\kappa\sqrt{\zeta^2 - 1}\sqrt{(r_b r_a + \mathbf{x}_b\mathbf{x}_a)/2}\right] e^{-\kappa\zeta(r_b + r_a)}. \quad (13.53)$$

13.3 Absence of Time Slicing Corrections for $D = 2$

We now convince ourselves that the finite thickness of the pseudotime slices in the intermediate formulas does not change the time evolution amplitude obtained in the last section [6]. The reader who is unaware of the historic difficulties which had to be overcome may not be interested in the upcoming technical discussion. He may skip this section and be satisfied with a brief argument given in Section 13.6.

The potential term in the action (13.9) can be ignored since it is of order ϵ_s and the time slicing can only produce higher than linear correction terms in ϵ_s which do not contribute in the continuum limit $\epsilon_s \to 0$. The crucial point where corrections might enter is in the transformation of the measure and the pseudotime-sliced kinetic terms in (13.8), (13.9). In vector notation, the coordinate transformation reads, at every time slice n,

$$\mathbf{x}_n = A(\mathbf{u}_n)\mathbf{u}_n. \tag{13.54}$$

Among the equivalent possibilities offered in Section 11.2 to transform a time-sliced path integral we choose the Taylor expansion (11.56) to map $\Delta\mathbf{x}$ into $\Delta\mathbf{u}$. After inserting (13.15) into (11.56) we find

$$\Delta x^i = 2A^i{}_\mu(\mathbf{u})\Delta u^\mu - \partial_\nu A^i{}_\mu(\mathbf{u})\Delta u^\mu \Delta u^\nu. \tag{13.55}$$

Since the mapping $\mathbf{x}(\mathbf{u})$ is quadratic in $\mathbf{u}$, there are no higher-order expansion terms. Note that due to the absence of curvature and torsion in the $\mathbf{u}$-space, the coordinate transformation is holonomic and $\Delta\mathbf{x}$ can also be calculated directly from $\mathbf{x}(\mathbf{u}) - \mathbf{x}(\mathbf{u} - \Delta\mathbf{u})$. Indeed, using the linearity of $A(\mathbf{u})$ in $\mathbf{u}$, we find from (13.54)

$$\Delta\mathbf{x}_n = A(\mathbf{u}_n)\mathbf{u}_n - A(\mathbf{u}_{n-1})\mathbf{u}_{n-1} = 2A(\mathbf{u}_n - \tfrac{1}{2}\Delta\mathbf{u}_n)\Delta\mathbf{u}_n = 2A(\bar{\mathbf{u}}_n)\Delta\mathbf{u}_n, \tag{13.56}$$

where $\bar{\mathbf{u}}_n$ is average across the slice. The Taylor expansion of $A(\mathbf{u}_n - \frac{1}{2}\Delta\mathbf{u}_n)$ has only two terms and leads to (13.55).

Using (13.56) we can write

$$(\Delta\mathbf{x}_n)^2 = 4\bar{\mathbf{u}}_n^2(\Delta\mathbf{u}_n)^2, \tag{13.57}$$

$$\bar{\mathbf{u}}_n \equiv (\mathbf{u}_n + \mathbf{u}_{n-1})/2. \tag{13.58}$$

The kinetic term of the short-time action in the nth time slice of Eq. (13.9) therefore becomes

$$\mathcal{A}^\epsilon = \frac{M}{2\epsilon_s}\frac{(\Delta\mathbf{x}_n)^2}{r_n^{1-\lambda}r_{n-1}^\lambda} = \frac{M}{2\epsilon_s}\frac{4\bar{\mathbf{u}}_n^2}{(\mathbf{u}_n^2)^{1-\lambda}(\mathbf{u}_{n-1}^2)^\lambda}(\Delta\mathbf{u}_n)^2. \tag{13.59}$$

This is expanded around the postpoint and yields

$$\bar{\mathbf{u}}_n = \mathbf{u}_n - \frac{1}{2}\Delta\mathbf{u}_n, \tag{13.60}$$

$$\mathbf{u}_{n-1} = \mathbf{u}_n - \Delta\mathbf{u}_n, \tag{13.61}$$

$$\frac{\bar{\mathbf{u}}_n^2}{(\mathbf{u}_n^2)^{1-\lambda}(\mathbf{u}_{n-1}^2)^\lambda} = 1 + (2\lambda - 1)\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2} + \left(\frac{1}{4} - \lambda\right)\frac{\Delta{\mathbf{u}_n}^2}{\mathbf{u}_n^2} + 2\lambda^2\left(\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2}\right)^2. \tag{13.62}$$

It is useful to separate the short-time action into a leading term

$$\mathcal{A}_0^\epsilon(\Delta\mathbf{u}_n) = 4M\frac{(\Delta\mathbf{u}_n)^2}{2\epsilon_s}, \tag{13.63}$$

plus correction terms

$$\Delta\mathcal{A}^\epsilon = 4M\frac{(\Delta\mathbf{u}_n)^2}{2\epsilon_s} \times \left[(2\lambda-1)\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2} + \left(\frac{1}{4}-\lambda\right)\frac{\Delta{\mathbf{u}_n}^2}{\mathbf{u}_n^2} + 2\lambda^2\left(\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2}\right)^2\right], \tag{13.64}$$

which will be treated perturbatively.

In order to perform the transformation of the measure of integration in (13.8), we expand $\Delta\mathbf{x}$ accordingly:

$$\begin{aligned}\Delta x^i &= 2{A^i}_\mu(\mathbf{u}-\frac{1}{2}\Delta\mathbf{u})\Delta u^\mu \\ &= 2{A^i}_\mu(\mathbf{u})\Delta u^\mu - \partial_\nu {A^i}_\mu(\mathbf{u})\Delta u^\mu\Delta u^\nu.\end{aligned} \tag{13.65}$$

The indices n have been suppressed, for brevity. This expression has, of course, the general form (10.96), after inserting there

$$e^i{}_\mu(\mathbf{u}) = 2{A^i}_\mu(\mathbf{u}). \tag{13.66}$$

Since the transformation matrix ${A^i}_\mu(\mathbf{u})$ in (13.15) is linear in $\mathbf{u}$, the matrix $e^i{}_\mu(\mathbf{u})$ has no second derivatives, and the Jacobian action (11.60) and (10.145) reduce to

$$\begin{aligned}\frac{i}{\hbar}\mathcal{A}_J^\epsilon &= -e_i{}^\mu e^i{}_{\{\mu,\nu\}}\Delta u^\nu - \frac{1}{2}e_i{}^\mu e^i{}_{\{\kappa,\nu\}}e_j{}^\kappa e^j{}_{\mu,\lambda}\Delta u^\nu\Delta u^\lambda \\ &= -\Gamma_{\{\nu\mu\}}{}^\mu\Delta u^\nu - \frac{1}{2}\Gamma_{\{\nu\kappa\}}{}^\mu\Gamma_{\{\mu\lambda\}}{}^\kappa\Delta u^\nu\Delta u^\lambda.\end{aligned} \tag{13.67}$$

The expansion coefficients are easily calculated using the reciprocal basis dyad

$$e_i{}^\kappa = \frac{1}{2\mathbf{u}^2}e^i{}_\kappa, \tag{13.68}$$

as

$$\begin{aligned}\Gamma_{\nu\mu}{}^\mu &= e_i{}^\mu\partial_\nu e^i{}_\mu = \frac{2u^\nu}{\mathbf{u}^2}, \\ \Gamma_{\mu\nu}{}^\mu &= -e^i{}_\nu\partial_\mu e_i{}^\mu = \frac{2u^\nu}{\mathbf{u}^2}, \\ \Gamma_{\nu\kappa}{}^\mu\Gamma_{\lambda\mu}{}^\kappa &= -\partial_\lambda e_i{}^\kappa\partial_\nu e^i{}_\kappa = -\frac{2}{\mathbf{u}^4}(\delta^{\nu\lambda}\mathbf{u}^2 - 2u^\nu u^\lambda).\end{aligned} \tag{13.69}$$

The second equation is found directly from

$$-\partial_\mu e_i{}^\mu = -\partial_\mu(2\mathbf{u}^2)^{-1}e^i{}_\mu = e_i{}^\mu\ 2u^\mu\mathbf{u}^{-2}, \tag{13.70}$$

which, in turn, follows from the obvious identity $\partial_\mu e^i{}_\mu = 0$. Note that the third expression in (13.69) is automatically equal to $\Gamma_{\{\nu\kappa\}}{}^\sigma\Gamma_{\{\lambda\sigma\}}{}^\kappa$, i.e., of the form required in (13.67), since the u^μ-space has no torsion and $\Gamma_{\nu\kappa}{}^\sigma = \Gamma_{\kappa\nu}{}^\sigma$. After inserting Eqs. (13.69) into the right-hand side of (13.67), we find the postpoint expansion

$$\frac{i}{\hbar}\mathcal{A}_J^\epsilon = -\left[2\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2} - \frac{\Delta{\mathbf{u}_n}^2}{\mathbf{u}_n^2} + 2\left(\frac{\mathbf{u}\Delta\mathbf{u}_n}{\mathbf{u}_n^2}\right)^2 + \dots\right]. \tag{13.71}$$

The measure of integration in (13.8) contains additional factors r_b, r_n, r_a which require a further treatment. First we rewrite it as

$$\begin{aligned}\frac{(r_b/r_a)^{2\lambda-1}}{2\pi i\epsilon_s\hbar}\prod_{n=1}^N\left[\int\frac{d^2\Delta x_n}{2\pi i\epsilon_s r_{n-1}/M}\right] &\approx \frac{1}{2\pi i\epsilon_s\hbar}\prod_{n=1}^N\left[\int\frac{d^2\Delta x_n}{2\pi i\epsilon_s\hbar r_n/M}\right]\prod_{n=1}^{N+1}\left(\frac{r_n}{r_{n-1}}\right)^{2\lambda} \\ &= \frac{1}{2\pi i\epsilon_s\hbar}\prod_{n=2}^{N+1}\left[\int\frac{d^2\Delta x_n}{2\pi i\epsilon_s\hbar r_n/M}\right]e^{i\mathcal{A}_f^N/\hbar}.\end{aligned} \tag{13.72}$$

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 $\prod_{n=2}^{N+1}\int d^2\Delta x_n = \prod_{n=1}^{N}\int d^2\Delta x_n$. In the first expression on the right-hand side we have further shifted the subscripts of the factors $1/r_{n-1}$ in the integral measure from $n-1$ to n and compensated for this by an overall factor $\prod_{n=1}^{N+1}(r_n/r_{n-1})$. Together with the prefactor $(r_b/r_a)^{2\lambda-1}$, this can be expressed as a product $\prod_{n=1}^{N+1}(r_n/r_{n-1})^{2\lambda}$. There is only a negligible error of order ϵ_s^2 at the upper end [this being the reason for writing the symbol $\approx$ rather than $=$ in (13.72)]. In the last part of the equation we have introduced an effective action

$$\mathcal{A}_f^N \equiv \sum_{n=1}^{N+1} \mathcal{A}_f^\epsilon \tag{13.73}$$

due to the $(r_n/r_{n-1})^{2\lambda}$ factors, with

$$\frac{i}{\hbar}\mathcal{A}_f^\epsilon = 2\lambda \log \frac{r_n^2}{r_{n-1}^2} = 2\lambda \log \frac{\mathbf{u}_n^2}{\mathbf{u}_{n-1}^2}. \tag{13.74}$$

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

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

$$d^2\Delta x = 4\mathbf{u}^2 d^2\Delta u \;\exp\left(\frac{i}{\hbar}\mathcal{A}_J^\epsilon\right). \tag{13.75}$$

The measure becomes

$$\frac{1}{2}\times\frac{4}{2\cdot 2\pi i\epsilon_s\hbar}\prod_{n=1}^{N}\left[\int\frac{4d^2\Delta u_n}{2\cdot 2\pi i\epsilon_s\hbar/M}\right]\exp\left[\frac{i}{\hbar}(\mathcal{A}_J^N+\mathcal{A}_f^N)\right], \tag{13.76}$$

where $\mathcal{A}_J^N$ is the sum over all time-sliced Jacobian action terms $\mathcal{A}_J^\epsilon$ of (13.71):

$$\mathcal{A}_J^N \equiv \sum_{n=1}^{N+1}\mathcal{A}_J^\epsilon. \tag{13.77}$$

The extra factors 2 in the measure denominators of (13.76) are introduced to let the $\mathbf{u}_n$-integrations run over the entire $\mathbf{u}$-space, in which case the $\mathbf{x}$-space is traversed twice.

The time-sliced expression (13.76) has an important feature which was absent in the continuous formulation. It receives dominant contributions not only from the region neighborhood $\mathbf{u}_n \sim \mathbf{u}_{n-1}$, in which case $(\Delta\mathbf{u}_n)^2$ is of order ϵ_s, but also from $\mathbf{u}_n \sim -\mathbf{u}_{n-1}$ where $(\bar{\mathbf{u}}_n)^2$ is of order ϵ_s. This is understandable since both configurations correspond to $\mathbf{x}_n$ being close to $\mathbf{x}_{n-1}$ and must be included. Fortunately, for symmetry reasons, they give identical contributions so that we need to discuss only the case $\mathbf{u}_n \sim \mathbf{u}_{n-1}$, the contribution from the second case being simply included by dropping the factors 2 in the measure denominators.

To process the measure further, we expand the action $\mathcal{A}_f^\epsilon$ (13.76) around the postpoint and find

$$\frac{i}{\hbar}\mathcal{A}_f^\epsilon \;=\; 2\lambda\log\left(\frac{\mathbf{u}_n^2}{\mathbf{u}_{n-1}^2}\right) = 2\lambda\left[2\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2} - \frac{\Delta\mathbf{u}_n{}^2}{\mathbf{u}_n^2} + 2\left(\frac{\mathbf{u}\Delta\mathbf{u}_n}{\mathbf{u}_n^2}\right)^2 + \dots\right]. \tag{13.78}$$

A comparison with (13.71) shows that adding $(i/\hbar)\mathcal{A}_f^\epsilon$ and $(i/\hbar)\mathcal{A}_J^\epsilon$ merely changes 2λ in $\mathcal{A}_f^\epsilon$ into $2\lambda-1$.

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

$$\mathcal{A}^\epsilon = \mathcal{A}_0^\epsilon + \Delta_{\rm corr}\mathcal{A}^\epsilon, \tag{13.79}$$

with the leading free-particle action

$$\mathcal{A}_0^\epsilon(\Delta\mathbf{u}_n) = 4M\frac{(\Delta\mathbf{u}_n)^2}{2\epsilon_s}, \tag{13.80}$$

and the total correction term

$$\begin{aligned}\frac{i}{\hbar}\Delta_{\rm corr}\mathcal{A}^\epsilon &\equiv \frac{i}{\hbar}(\Delta\mathcal{A}^\epsilon + \mathcal{A}_J^\epsilon + \mathcal{A}_f^\epsilon)\\ &= \frac{i}{\hbar}4M\frac{\Delta\mathbf{u}_n{}^2}{2\epsilon_s}\left[(2\lambda-1)\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2} + \left(\frac{1}{4}-\lambda\right)\frac{\Delta\mathbf{u}_n{}^2}{\mathbf{u}_n^2} + 2\lambda^2\left(\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2}\right)^2\right]\\ &\quad + (2\lambda-1)\left[2\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2} - \frac{\Delta\mathbf{u}_n{}^2}{\mathbf{u}_n^2} + 2\left(\frac{\mathbf{u}_n\Delta\mathbf{u}_n}{\mathbf{u}_n^2}\right)^2\right] + \dots\ .\end{aligned} \tag{13.81}$$

We now show that the action $\Delta_{\rm corr}\mathcal{A}^\epsilon$ is equivalent to zero by proving that the kernel associated with the short-time action

$$K^\epsilon(\Delta\mathbf{u}) = \frac{4}{2\cdot 2\pi i\epsilon_s\hbar/M}\exp\left[\frac{i}{\hbar}(\mathcal{A}_0^\epsilon + \Delta_{\rm corr}\mathcal{A}^\epsilon)\right] \tag{13.82}$$

is equivalent to the zeroth-order free-particle kernel

$$K_0^\epsilon(\Delta\mathbf{u}) = \frac{4}{2\cdot 2\pi i\epsilon_s\hbar/M}\exp\left[\frac{i}{\hbar}\mathcal{A}_0^\epsilon\right]. \tag{13.83}$$

The equivalence is established by checking the equivalence relations (11.71) and (11.72). For the kernel (13.82), the correction (11.71) is

$$C_1 = C \equiv \exp\left(\frac{i}{\hbar}\Delta_{\rm corr}\mathcal{A}^\epsilon\right) - 1. \tag{13.84}$$

It has to be compared with the trivial factor of the kernel (13.83):

$$C_2 = 0. \tag{13.85}$$

Thus, the equivalence requires showing that

$$\begin{aligned}\langle C\rangle_0 &= 0,\\ \langle C\ (\mathbf{p}\Delta\mathbf{u})\rangle_0 &= 0.\end{aligned} \tag{13.86}$$

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

$$\langle\Delta u^\mu\Delta u^\nu\rangle_0 \equiv \frac{i\hbar\epsilon_s}{4M}\delta^{\mu\nu}, \tag{13.87}$$

$$\langle\Delta u^{\mu_1}\cdots\Delta u^{\mu_{2n}}\rangle_0 = \left(\frac{i\hbar\epsilon_s}{4M}\right)^n\delta^{\mu_1\dots\mu_{2n}}, \quad n>1, \tag{13.88}$$

where the contraction tensors $\delta^{\mu_1\cdots\mu_{2n}}$ of Eq. (8.64), determined recursively from

$$\delta^{\mu_1\cdots\mu_{2n}} \equiv \delta^{\mu_1\mu_2}\delta^{\mu_3\mu_4\cdots\mu_{2n}} + \delta^{\mu_1\mu_3}\delta^{\mu_2\mu_4\cdots\mu_{2n}} + \dots + \delta^{\mu_1\mu_{2n}}\delta^{\mu_2\mu_3\cdots\mu_{2n-1}}. \tag{13.89}$$

They consist of $(2n-1)!!$ products of pair contractions $\delta^{\mu_i\mu_j}$. More specifically, we encounter, in calculating (13.86), expectations of the type

$$\langle(\Delta\mathbf{u})^{2k}(\mathbf{u}\Delta\mathbf{u})^{2l}\rangle_0 = \left(\frac{i\hbar\epsilon_s}{4M}\right)^{k+l}\frac{[D+2(k+l-1)]!!}{(D+2l-2)!!}(2l-1)!!(\mathbf{u}^2)^l, \tag{13.90}$$

and

$$\langle(\Delta\mathbf{u})^{2k}(\mathbf{u}\Delta\mathbf{u})^{2l}(\mathbf{u}\Delta\mathbf{u})(\mathbf{p}\Delta\mathbf{u})\rangle_0 = \left(\frac{i\hbar\epsilon_s}{4M}\right)^{k+l+1}\frac{[D+2(k+l)]!!}{(D+2l)!!}(2l-1)!!(\mathbf{up}), \tag{13.91}$$

where we have allowed for a general $\mathbf{u}$-space dimension D. Expanding (13.86) we now check that, up to first order in ϵ_s, the expectations $\langle C\rangle_0$ and $\langle C\ (\mathbf{p}\Delta\mathbf{u})\rangle_0$ vanish:

$$\langle C\rangle_0 = \frac{i}{\hbar}\langle\Delta_{\rm corr}\mathcal{A}^\epsilon\rangle_0 + \frac{1}{2!}\left(\frac{i}{\hbar}\right)^2\langle(\Delta_{\rm corr}\mathcal{A}^\epsilon)^2\rangle_0 \;=\; 0, \tag{13.92}$$

$$\langle C\ (\mathbf{p}\Delta\mathbf{u})\rangle_0 = \frac{i}{\hbar}\langle\Delta_{\rm corr}\mathcal{A}^\epsilon\ (\mathbf{p}\Delta\mathbf{u})\rangle_0 \;=\; 0. \tag{13.93}$$

Indeed, the first term in (13.92) becomes

$$\frac{i}{\hbar}\langle\Delta_{\rm corr}\mathcal{A}^\epsilon\rangle_0 = 2i\frac{\hbar\epsilon_s}{M}\left[-\left(\frac{1}{4}-\lambda\right)\frac{(D+2)D}{16} - 2\lambda^2\frac{D+2}{16}\right], \tag{13.94}$$

and reduces for $D=2$ to

$$\frac{i}{\hbar}\langle\Delta_{\rm corr}\mathcal{A}^\epsilon\rangle_0 = -i\frac{\hbar\epsilon_s}{M}\left(\lambda-\frac{1}{2}\right)^2. \tag{13.95}$$

This is canceled identically in λ by the second term in (13.92), which is equal to

$$\frac{1}{2!}\left(\frac{i}{\hbar}\right)^2\langle(\Delta_{\rm corr}\mathcal{A}^\epsilon)^2\rangle_0 = \frac{i}{2}\frac{\hbar\epsilon_s}{M}\left[4(2\lambda-1)^2\frac{(D+4)(D+2)}{64} + 4(2\lambda-1)^2\frac{1}{4} - 8(2\lambda-1)^2\frac{D+2}{16}\right], \tag{13.96}$$

and reduces for $D=2$ to

$$\frac{1}{2!}\left(\frac{i}{\hbar}\right)^2\langle(\Delta_{\rm corr}\mathcal{A}^\epsilon)^2\rangle_0 = i\frac{\hbar\epsilon_s}{M}\left(\lambda-\frac{1}{2}\right)^2. \tag{13.97}$$

Similarly, the expectation (13.93),

$$\langle\Delta_{\rm corr}\mathcal{A}^\epsilon\ (\mathbf{p}\Delta\mathbf{u})\rangle_0 = -\frac{\hbar^2\epsilon_s}{4M}[(2\lambda-1)(D+2)/4-(2\lambda-1)], \tag{13.98}$$

is seen to vanish identically in λ for $D=2$.

Thus there is no finite time slicing correction to the naive transformation formula (13.34) for the Coulomb path integral in two dimensions.

13.4 Solution for the Three-Dimensional Coulomb System

We now turn to the physically relevant Coulomb system in three dimensions. The first problem is to find again some kind of "square root" coordinates to convert the potential $-Er$ in the pseudotime Hamiltonian in the exponent of Eq. (13.5) into a harmonic potential. In two dimensions, the answer was a complex square root. Here, it is a "quaternionic square root" known as the *Kustaanheimo-Stiefel transformation*, which was used extensively in celestial mechanics [7]. To apply this transformation, the three-vectors $\mathbf{x}$ must first be mapped into a four-dimensional u^μ-space ($\mu = 1,2,3,4$) via the equations

$$x^i = \bar{z}\sigma^i z, \qquad r = \bar{z}z. \tag{13.99}$$

Here σ^i are the Pauli matrices (1.448), and $z, \bar{z}$ the two-component objects

$$z = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}, \quad \bar{z} = (z_1^*, z_2^*), \tag{13.100}$$

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

$$z_1 = (u^1 + iu^2), \quad z_2 = (u^3 + iu^4). \tag{13.101}$$

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

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

In Eqs. (13.99), the angle γ obviously cancels. Each point in $\mathbf{x}$-space corresponds to an entire curve in u^μ-space along which the angle γ runs through the interval $[0, 4\pi]$.

We can write (13.99) also in a matrix form

$$\begin{pmatrix} x^1 \\ x^2 \\ x^3 \end{pmatrix} = A(\vec{u}) \begin{pmatrix} u^1 \\ u^2 \\ u^3 \\ u^4 \end{pmatrix}, \tag{13.102}$$

with the 3×4 matrix

$$A(\vec{u}) = \begin{pmatrix} u^3 & u^4 & u^1 & u^2 \\ u^4 & -u^3 & -u^2 & u^1 \\ u^1 & u^2 & -u^3 & -u^4 \end{pmatrix}. \tag{13.103}$$

Since

$$r = (u^1)^2 + (u^2)^2 + (u^3)^2 + (u^4)^2 \equiv (\vec{u})^2, \tag{13.104}$$

this transformation certainly makes the potential $-Er$ in the pseudotime Hamiltonian harmonic in $\vec{u}$. The arrow on top indicates the four-vector nature of u^μ.

Consider now the kinetic term $\int ds(M/2r)(d\mathbf{x}/ds)^2$ in the action (13.10). Each path $\mathbf{x}(s)$ is associated with an infinite set of paths $\vec{u}(s)$ in $\vec{u}$-space, depending on the choice of a dummy path $\gamma(s)$ in parameter space. The mapping of the tangent vectors du^μ into dx^i is given by

$$\begin{pmatrix} dx^1 \\ dx^2 \\ dx^3 \end{pmatrix} = 2 \begin{pmatrix} u^3 & u^4 & u^1 & u^2 \\ u^4 & -u^3 & -u^2 & u^1 \\ u^1 & u^2 & -u^3 & -u^4 \end{pmatrix} \begin{pmatrix} du^1 \\ du^2 \\ du^3 \\ du^4 \end{pmatrix}. \tag{13.105}$$

To make the mapping unique we must prescribe at least some differential equation for the dummy angle $d\gamma$. This is done most simply by replacing $d\gamma$ by a parameter which is more naturally related to the components dx^i on the left-hand side. We embed the tangent vector (dx^1, dx^2, dx^3) into a fictitious four-dimensional space and define a new, fourth component dx^4 by an additional fourth row in the matrix $A(\vec{u})$, thereby extending (13.29) to the four-vector equation

$$d\vec{x} = 2A(\vec{u})d\vec{u}. \tag{13.106}$$

The arrow on top of x indicates that x has become a four-vector. For symmetry reasons, we choose the 4×4 matrix $A(\vec{u})$ as

$$A(\vec{u}) = \begin{pmatrix} u^3 & u^4 & u^1 & u^2 \\ u^4 & -u^3 & -u^2 & u^1 \\ u^1 & u^2 & -u^3 & -u^4 \\ u^2 & -u^1 & u^4 & -u^3 \end{pmatrix}. \tag{13.107}$$

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

$$\begin{aligned} dx^4 &= 2(u^2du^1 - u^1du^2 + u^4du^3 - u^3du^4) \\ &= r(\cos\theta\; d\varphi + d\gamma). \end{aligned} \tag{13.108}$$

Now we make the important observation that this relation is not integrable since $\partial x^4/\partial u^1 = 2u^2$, $\partial x^4/\partial u^2 = -2u^1$, and hence

$$(\partial_{u^1}\partial_{u^2} - \partial_{u^2}\partial_{u^1})x^4(u^\mu) = -4, \qquad (\partial_{u^3}\partial_{u^4} - \partial_{u^4}\partial_{u^3})x^4(u^\mu) = -4, \tag{13.109}$$

implying that $x^4(u^\mu)$ does not satisfy the integrability criterion of Schwarz [recall (10.19)]. The mapping is nonholonomic and 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 the next section. The impossibility of finding a unique mapping between the *points* of $\vec{x}$- and $\vec{u}$-space has the consequence that the mapping between *paths* is multivalued with respect to the initial point. After having chosen a specific image for the initial point, the mapping (13.107) determines the image path uniquely.

We now incorporate the dummy fourth dimension into the action by replacing $\mathbf{x}$ in the kinetic term by the four-vector $\vec{x}$ and extending the kinetic action to

$$\mathcal{A}^N_{\rm kin} \equiv \sum_{n=1}^{N+1} \frac{M}{2} \frac{(\vec{x}_n - \vec{x}_{n-1})^2}{\epsilon_s r_n^{1-\lambda} r_{n-1}^\lambda}. \tag{13.110}$$

The additional contribution of the fourth components $x^4_n - x^4_{n-1}$ can be eliminated trivially from the final pseudotime evolution amplitude by integrating each time slice over dx^4_{n-1} with the measure

$$\prod_{n=1}^{N+1} \int_{-\infty}^{\infty} \frac{d(\Delta x^4)_n}{\sqrt{2\pi i\epsilon_s\hbar r_n^{1-\lambda} r_{n-1}^\lambda/M}}. \tag{13.111}$$

Note that in these integrals, the radial coordinates r_n are fixed numbers. In contrast to the spatial integrals d^3x_{n-1}, the fourth coordinate must be integrated also over the initial auxiliary coordinate $x_0^4 = x_a^4$. Thus we use the trivial identity

$$\prod_{n=1}^{N+1}\left[\int_{-\infty}^{\infty}\frac{d(\Delta x^4)_n}{\sqrt{2\pi i\epsilon_s\hbar r_n^{1-\lambda}r_{n-1}^{\lambda}/M}}\right]\exp\left[\frac{i}{\hbar}\sum_{n=1}^{N+1}\frac{M}{2}\frac{(\Delta x_n^4)^2}{\epsilon_s r_n^{1-\lambda}r_{n-1}^{\lambda}}\right] = 1. \tag{13.112}$$

Hence the pseudotime evolution amplitude of the Coulomb system in three dimensions can be rewritten as the four-dimensional path integral

$$\begin{aligned}\langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle &= \int dx_a^4\frac{r_b^{\lambda}r_a^{1-\lambda}}{(2\pi i\epsilon_s\hbar r_b^{1-\lambda}r_a^{\lambda}/M)^2}\\ &\times\prod_{n=2}^{N+1}\left[\int_{-\infty}^{\infty}\frac{d^4\Delta x_n}{(2\pi i\epsilon_s\hbar r_{n-1}/M)^2}\right]\exp\left(\frac{i}{\hbar}\mathcal{A}_E^N\right),\end{aligned} \tag{13.113}$$

where $\mathcal{A}_E^N$ is the action (13.9) in which the three-vectors $\mathbf{x}_n$ are replaced by the four-vectors $\vec{x}_n$, although r is still the length of the spatial part of $\vec{x}$. By distributing the factors r_b, r_n, r_a evenly over the intervals, shifting the subscripts n of the factors $1/r_n$ in the measure to $n+1$, and using the same procedure as in Eq. (13.72), we arrive at the pseudotime evolution amplitude

$$\begin{aligned}\langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle = \frac{1}{(2\pi\, i\epsilon_s\hbar/M)^2}\int_{-\infty}^{\infty}\frac{dx_a^4}{r_a}\\ \times\prod_{n=2}^{N+1}\left[\int\frac{d^4\Delta\vec{x}_n}{(2\pi i\epsilon_s\hbar r_n/M)^2}\right]\exp\left[\frac{i}{\hbar}(\mathcal{A}_E^N+\mathcal{A}_f^N)\right],\end{aligned} \tag{13.114}$$

with the sliced action

$$\mathcal{A}_E^N[\vec{x},\vec{x}'] = (N+1)\epsilon_s e^2 + \sum_{n=1}^{N+1}\left[\frac{M}{2}\frac{(\Delta\vec{x}_n)^2}{\epsilon_s r_n^{1-\lambda}\, r_{n-1}^{\lambda}} + \epsilon_s\, r_n^{1-\lambda}\, r_{n-1}^{\lambda}\, E\right]. \tag{13.115}$$

The action $\mathcal{A}_f^N$ accounts for all remaining factors in the integral measure. The prefactor is now $(r_b/r_a)^{3\lambda-2}$ and can be written as a product $\prod_1^{N+1}(r_n/r_{n-1})^{3\lambda-2}$. The index shift in the factor $1/r$ changes the power $3\lambda-2$ to 3λ

$$\frac{i}{\hbar}\mathcal{A}_f^N = 3\lambda\sum_{n=1}^{N+1}\log\left(\frac{\vec{u}_n^2}{\vec{u}_{n-1}^2}\right) \tag{13.116}$$

[compare (13.73)]. As in the two-dimensional case we shall at first ignore the subtleties due to the time slicing. Thus we set $\lambda = 0$ and apply the transformation formally to the continuum limit of the action $\mathcal{A}_E^N$, which has the form (13.10), except that $\mathbf{x}$ is replaced by $\vec{x}$. Using the properties of the matrix (13.107)

$$\begin{aligned}A^T &= \vec{u}^2 A^{-1},\\ \det A &= \sqrt{\det(AA^T)} = r^2,\end{aligned} \tag{13.117}$$

we see that

$$\vec{x}'^2 = 4\vec{u}^2\vec{u}'^2 = 4r\vec{u}'^2, \tag{13.118}$$
$$d^4x = 16r^2d^4u. \tag{13.119}$$

In this way, we find the formal relation

$$\langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle = e^{ie^2S/\hbar}\frac{1}{16}\int\frac{dx_a^4}{r_a}(\vec{u}_bS|\vec{u}_a0) \tag{13.120}$$

to the time evolution amplitude of the four-dimensional harmonic oscillator

$$(\vec{u}_bS|\vec{u}_a0) = \int\mathcal{D}^4u(s)\exp\left(\frac{i}{\hbar}\mathcal{A}_{\rm os}\right), \tag{13.121}$$

with the action

$$\mathcal{A}_{\rm os} = \int_0^S ds\frac{\mu}{2}(\vec{u}'^2 - \omega^2\vec{u}^2). \tag{13.122}$$

The parameters are, as in (13.27) and (13.28),

$$\mu = 4M, \quad \omega = \sqrt{-E/2M}. \tag{13.123}$$

The relation (13.120) is the analog of (13.31). Instead of a sum over the two images of each point $\mathbf{x}$ in $\mathbf{u}$-space, there is now an integral $\int dx_a^4/r_a$ over the infinitely many images in the four-dimensional $\vec{u}$-space. This integral can be rewritten as an integral over the third Euler angle γ using the relation (13.108). Since $\mathbf{x}$ and thus the polar angles θ, φ remain fixed during the integration, we have directly $\int dx_a^4/r_a = \int d\gamma_a$. As far as the range of integration is concerned, we observe that it may be restricted to a single period $\gamma_a \in [0, 4\pi]$. The other periods can be included in the oscillator amplitude. By specifying a four-vector $\vec{u_b}$, all paths are summed which run either to the final Euler angle γ_b or to all its periodic repetitions [which by (13.102) have the same $\vec{u_b}$]. This was the lesson learned in Section 6.1. Equation (13.120) contains, instead, a sum over all initial periods which is completely equivalent to this. Thus the relation (13.120) reads, more specifically,

$$\langle \mathbf{x}_b|\hat{\mathcal{U}}_E(S)|\mathbf{x}_a\rangle = e^{ie^2S/\hbar}\frac{1}{16}\int_0^{4\pi}d\gamma_a(\vec{u}_bS|\vec{u}_a0). \tag{13.124}$$

The reason why the other periods in (13.120) must be omitted can best be understood by comparison with the two-dimensional case. There we observed a two-fold degeneracy of contributions to the time-sliced path integral which cancel all factors 2 in the measure (13.76). Here the same thing happens except 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 all periods $\gamma_n \in [4\pi l, 4\pi(l+1)]$. This suggests that each volume element d^4u_n must be divided by an infinite factor to remove this degeneracy. However, this is not necessary since the gradient term produces precisely the same infinite factor. Indeed,

$$(\vec{u}_n + \vec{u}_{n-1})^2(\vec{u}_n - \vec{u}_{n-1})^2 \tag{13.125}$$

is small for $\vec{x}_n \approx \vec{x}_{n-1}$ at infinitely many places of $\gamma_n - \gamma_{n-1}$, once for 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 this cancellation does not occur is in the integral $\int dx_a^4/r_a$. Here the infinite factor in the denominator is still present, but it can be removed by restricting the integration over γ_a in (13.124) to a single period [8].

Note 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 previous two-dimensional system.

The time-sliced path integral for the harmonic oscillator can, of course, be done immediately, the amplitude being the four-dimensional version of (13.33) [recall (2.177)]:

$$\begin{aligned}(\vec{u}_b S|\vec{u}_a 0) &= \frac{1}{(2\pi i\hbar\epsilon_s/\mu)^2}\prod_{n=1}^{N}\left[\int\frac{d^4\Delta u_n}{2\pi i\hbar\epsilon_s/\mu}\right]\exp\left[\frac{i}{\hbar}\sum_{n=1}^{N}\frac{\mu}{2}\left(\frac{1}{\epsilon_s}\Delta\vec{u}_n{}^2 - \epsilon_s\omega^2\vec{u}_n^2\right)\right]\\ &= \frac{\omega^2}{(2\pi i\hbar\sin\omega S\,/\mu)^2}\exp\left\{\frac{i}{2\hbar}\frac{\mu\omega}{\sin\omega S}[(\vec{u}_b{}^2+\vec{u}_a^2)\cos\omega S - 2\vec{u}_b\vec{u}_a]\right\}.\end{aligned} \tag{13.126}$$

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

$$(\mathbf{x}_b|\mathbf{x}_a)_E = \int_0^\infty dS e^{ie^2S/\hbar}\frac{1}{16}\int_0^{4\pi} d\gamma_a(\vec{u}_b S|\vec{u}_a 0). \tag{13.127}$$

Just like (13.35), the integral is written most conveniently in terms of the variables (13.38), (13.40), so that we obtain the fixed-energy amplitude of the three-dimensional Coulomb system

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

In order to perform the integral over dx_b^4, we now express $\vec{u}_b\vec{u}_a$ in terms of the polar angles

$$\begin{aligned}\vec{u}_b\vec{u}_a = \sqrt{r_b r_a}\,\{&\cos(\theta_b/2)\cos(\theta_a/2)\cos[(\varphi_b-\varphi_a+\gamma_b-\gamma_a)/2]\\ &+\sin(\theta_b/2)\sin(\theta_a/2)\cos[(\varphi_b-\varphi_a-\gamma_b+\gamma_a)/2]\}\,.\end{aligned} \tag{13.128}$$

A trigonometric rearrangement brings this to the form

$$\begin{aligned}\vec{u}_b\vec{u}_a = \sqrt{r_b r_a}\,\{&\cos[(\theta_b-\theta_a)/2]\cos[(\varphi_b-\varphi_a)/2]\cos[(\gamma_b-\gamma_a)/2]\\ &-\cos[(\theta_b+\theta_a)/2]\sin[(\varphi_b-\varphi_a)/2]\sin[(\gamma_b-\gamma_a)/2]\}\,,\end{aligned} \tag{13.129}$$

and further to

$$\vec{u}_b\vec{u}_a = \sqrt{(r_b r_a + \mathbf{x}_b\mathbf{x}_a)/2}\cos[(\gamma_b - \gamma_a + \beta)/2], \tag{13.130}$$

where β is defined by

$$\tan\frac{\beta}{2} = \frac{\cos[(\theta_b+\theta_a)/2]\sin[(\varphi_b-\varphi_a)/2]}{\cos[(\theta_b-\theta_a)/2]\cos[(\varphi_b-\varphi_a)/2]}, \tag{13.131}$$

or

$$\cos\frac{\beta}{2} = \cos\frac{\theta_b-\theta_a}{2}\cos\frac{\varphi_b-\varphi_a}{2}\sqrt{\frac{r_b r_a}{(r_b r_a + \mathbf{x}_b\mathbf{x}_a)/2}}. \tag{13.132}$$

The integral $\int_0^{4\pi} d\gamma_a$ can now be done at each fixed $\mathbf{x}$. This gives the fixed-energy amplitude of the Coulomb system [1, 9, 11, 10].

$$\begin{aligned}(\mathbf{x}_b|\mathbf{x}_a)_E &= -i\,\frac{M\kappa}{\pi\hbar}\int_0^1 d\varrho\frac{\varrho^{-\nu}}{(1-\varrho)^2}I_0\left(2\kappa\frac{2\sqrt{\varrho}}{1-\varrho}\sqrt{(r_b r_a + \mathbf{x}_b\mathbf{x}_a)/2}\right)\\ &\times\ \exp\left[-\kappa\frac{1+\varrho}{1-\varrho}(r_b+r_a)\right],\end{aligned} \tag{13.133}$$

where κ and ν are the same parameters as in Eqs. (13.40).

The integral converges only for $\nu < 1$, as in the two-dimensional case. It is again possible to write down another integral representation which converges for all $\nu \neq 1, 2, 3, \dots$ by changing the variables of integration to $\zeta \equiv (1+\varrho)/(1-\varrho)$ and transforming 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 $(\zeta-1)^{-\nu}$, the replacement rule is

$$\int_1^\infty d\zeta(\zeta-1)^{-\nu}\dots \to \frac{\pi e^{i\pi\nu}}{\sin\pi\nu}\int_C\frac{d\zeta}{2\pi i}(\zeta-1)^{-\nu}\dots\ . \tag{13.134}$$

This leads to the representation

$$\begin{aligned}(\mathbf{x}_b|\mathbf{x}_a)_E = -i\frac{M}{\pi\hbar}\frac{\kappa}{2}\frac{\pi e^{i\pi\nu}}{\sin\pi\nu}\int_C\frac{d\zeta}{2\pi i}(\zeta-1)^{-\nu}(\zeta+1)^{\nu}\\ \times I_0(2\kappa\sqrt{\zeta^2-1}\sqrt{(r_b r_a+\mathbf{x}_b\mathbf{x}_a)/2})e^{-\kappa\zeta(r_b+r_a)}.\end{aligned} \tag{13.135}$$

13.5 Absence of Time Slicing Corrections for $D = 3$

Let us now prove that for the three-dimensional Coulomb system also, the finite time-slicing procedure does not change the formal result of the last section. The reader not interested in the details is again referred to the brief argument in Section 13.6. The action $\mathcal{A}_E^N$ in the time-sliced path integral has to be supplemented, in each slice, by the Jacobian action [as in (13.67)]

$$\begin{aligned}\frac{i}{\hbar}\mathcal{A}_J^\epsilon &= -e^\mu e^i{}_{\{\mu,\nu\}}\Delta u^\nu - e_i{}^\mu e^i{}_{\{\kappa,\nu\}}e_j{}^\kappa e^i{}_{\{\mu,\lambda\}}\Delta u^\nu\Delta u^\lambda\\ &= -\Gamma_{\{\nu\mu\}}{}^\mu\Delta u^\nu - \frac{1}{2}\Gamma_{\{\nu\kappa\}}{}^\sigma\Gamma_{\{\lambda\sigma\}}{}^\kappa\Delta u^\nu\Delta u^\lambda.\end{aligned} \tag{13.136}$$

The basis tetrad

$$e^i{}_\mu = \partial x^i/\partial u^\mu = 2A^i{}_\mu(\vec{u}), \quad i = 1, 2, 3, 4, \tag{13.137}$$

is now given by the 4×4 matrix (13.107), with the reciprocal tetrad

$$e_i{}^\mu = \frac{1}{2\vec{u}^2} e^i{}_\mu. \tag{13.138}$$

From this we find the matrix components of the connection [compare (13.18)]

$$\begin{aligned}
(\Gamma_1)_\mu{}^\nu &= \frac{1}{\vec{u}^2}\begin{pmatrix} u^1 & u^2 & -u^3 & -u^4 \\ -u^2 & u^1 & -u^4 & u^3 \\ u^3 & u^4 & u^1 & u^2 \\ u^4 & -u^3 & -u^2 & u^1 \end{pmatrix}_\mu^{\ \nu}, \\
(\Gamma_2)_\mu{}^\nu &= \frac{1}{\vec{u}^2}\begin{pmatrix} u^2 & -u^1 & u^4 & -u^3 \\ u^1 & u^2 & -u^3 & -u^4 \\ -u^4 & u^3 & u^2 & -u^1 \\ u^3 & u^4 & u^1 & u^2 \end{pmatrix}_\mu^{\ \nu}, \\
(\Gamma_3)_\mu{}^\nu &= \frac{1}{\vec{u}^2}\begin{pmatrix} u^3 & u^4 & u^1 & u^2 \\ -u^4 & u^3 & u^2 & -u^1 \\ -u^1 & -u^2 & u^3 & u^4 \\ -u^2 & u^1 & -u^4 & u^3 \end{pmatrix}_\mu^{\ \nu}, \\
(\Gamma_4)_\mu{}^\nu &= \frac{1}{\vec{u}^2}\begin{pmatrix} u^4 & -u^3 & -u^2 & u^1 \\ u^3 & u^4 & u^1 & u^2 \\ u^2 & -u^1 & u^4 & -u^3 \\ -u^1 & -u^2 & u^3 & u^4 \end{pmatrix}_\mu^{\ \nu}.
\end{aligned} \tag{13.139}$$

As in the two-dimensional case [see Eq. (13.19)], the connection satisfies the important identity

$$\Gamma_\mu{}^{\mu\nu} \equiv 0, \tag{13.140}$$

which is again a consequence of the relation [compare (13.21)]

$$\partial_\mu e^i{}_\mu = 0. \tag{13.141}$$

In Section 13.6, this will be shown to be the essential reason for the absence of the time slicing corrections being proved in this section.

However, there is now an important difference with respect to the two-dimensional case. The present mapping $dx^i = e^i{}_\mu(u)du^\mu$ is not integrable. Taking the antisymmetric part of $\Gamma_{\mu\nu}{}^\lambda$ we find the u^μ-space to carry a torsion $S_{\mu\nu}{}^\lambda$ whose only nonzero components are

$$S_{12}{}^\lambda = S_{34}{}^\lambda = \frac{1}{\vec{u}^2}(-u^2, u^1, -u^4, u^3)^\lambda. \tag{13.142}$$

The once-contracted torsion is

$$S_\mu = S_{\mu\nu}{}^\nu = \frac{u^\mu}{\vec{u}^2}. \tag{13.143}$$

For this reason, the contracted connections

$$\begin{aligned}
\Gamma_{\nu\mu}{}^\mu &= e_i{}^\mu \partial_\nu e^i{}_\mu = \frac{4u^\nu}{\vec{u}^2}, \\
\Gamma_{\mu\nu}{}^\mu &= -e^i{}_\nu \partial_\mu e_i{}^\mu = \frac{2u^\nu}{\vec{u}^2}
\end{aligned} \tag{13.144}$$

are no longer equal, as they were in (13.69). Symmetrization in the lower indices gives

$$\Gamma_{\{\nu\mu\}}{}^{\mu} = \frac{3u^{\nu}}{\vec{u}^2}. \tag{13.145}$$

Due to this, the $\Delta u^{\nu}\Delta u^{\lambda}$-terms in (13.136) are, in contrast to the two-dimensional case, not given directly by

$$\Gamma_{\nu\kappa}{}^{\sigma}\Gamma_{\lambda\sigma}{}^{\kappa} = -\frac{4}{\vec{u}^4}(\delta^{\nu\lambda}\vec{u}^2 - 2u^{\nu}u^{\lambda}). \tag{13.146}$$

The symmetrization in the lower indices is necessary and yields

$$\begin{aligned}\Gamma_{\{\nu\kappa\}}{}^{\sigma}\Gamma_{\{\lambda\sigma\}}{}^{\kappa} &= \Gamma_{\nu\kappa}{}^{\sigma}\Gamma_{\lambda\sigma}{}^{\kappa} - 2\Gamma_{\nu\kappa}{}^{\sigma}S_{\lambda\sigma}{}^{\kappa} + S_{\nu\kappa}{}^{\sigma}S_{\lambda\sigma}{}^{\kappa} \\ &= \Gamma_{\nu\kappa}{}^{\sigma}\Gamma_{\lambda\sigma}{}^{\kappa} - 2(-\delta_{\nu\lambda}\vec{u}^2 + 2u_{\nu}u_{\lambda})/\vec{u}^4 + u_{\nu}u_{\lambda}/\vec{u}^4.\end{aligned} \tag{13.147}$$

Collecting all terms, the Jacobian action (13.136) becomes

$$\frac{i}{\hbar}\mathcal{A}_J^{\epsilon} = -\left[3\frac{\vec{u}_n\Delta\vec{u}_n}{\vec{u}_n^2} - \frac{\Delta\vec{u}_n{}^2}{\vec{u}_n^2} + \frac{5}{2}\left(\frac{\vec{u}_n\Delta\vec{u}_n}{\vec{u}_n^2}\right)^2 + \dots\right]. \tag{13.148}$$

In contrast to the two-dimensional equation (13.71), this cannot be incorporated into $\mathcal{A}_f^{\epsilon}$. Although the two expressions contain the same terms, their coefficients are different [see (13.116)]:

$$\begin{aligned}\frac{i}{\hbar}\mathcal{A}_f^{\epsilon} &= 3\lambda\log\left(\frac{\vec{u}_n^2}{\vec{u}_{n-1}^2}\right) \\ &= 3\lambda\left[2\frac{\vec{u}_n\Delta\vec{u}_n}{\vec{u}_n^2} - \frac{\Delta\vec{u}_n{}^2}{\vec{u}_n^2} + 2\left(\frac{\vec{u}\Delta\vec{u}_n}{\vec{u}_n^2}\right)^2 + \dots\right].\end{aligned} \tag{13.149}$$

It is then convenient to rewrite (omitting the subscripts n)

$$\begin{aligned}\frac{i}{\hbar}\mathcal{A}_J^{\epsilon} &= -2\log\left[\frac{\vec{u}^2}{(\vec{u}-\Delta\vec{u})^2}\right] + \frac{\vec{u}\Delta\vec{u}}{\vec{u}^2} \\ &\quad -\frac{\Delta\vec{u}^2}{\vec{u}^2} + \frac{3}{2}\left(\frac{\vec{u}\Delta\vec{u}}{\vec{u}^2}\right)^2 + \dots\ ,\end{aligned} \tag{13.150}$$

and absorb the first term into $\mathcal{A}_f^{\epsilon}$, which changes 3λ to $(3\lambda - 2)$. Thus, we obtain altogether the additional action [to be compared with (13.81)]

$$\begin{aligned}\frac{i}{\hbar}\Delta_{\text{corr}}\mathcal{A}^{\epsilon} &= \frac{i}{\hbar}4M\frac{\Delta\vec{u}^2}{2\epsilon}\left[(2\lambda-1)\frac{\vec{u}\Delta\vec{u}}{\vec{u}^2} + (\frac{1}{4}-\lambda)\frac{\Delta\vec{u}^2}{\vec{u}^2} + 2\lambda^2\left(\frac{\vec{u}\Delta\vec{u}}{\vec{u}^2}\right)^2\right] \\ &\quad +(3\lambda-2)\left[2\frac{\vec{u}\Delta\vec{u}}{\vec{u}^2} - \frac{\Delta\vec{u}^2}{\vec{u}^2} + 2\left(\frac{\vec{u}\Delta\vec{u}}{\vec{u}^2}\right)^2\right] \\ &\quad +\frac{\vec{u}\Delta\vec{u}}{\vec{u}^2} - \frac{(\Delta\vec{u})^2}{\vec{u}^2} + \frac{3}{2}\left(\frac{\vec{u}\Delta\vec{u}}{\vec{u}^2}\right)^2 + \dots\ .\end{aligned} \tag{13.151}$$

Using this we now show that the expansion of the correction term

$$C = \exp\left(\frac{i}{\hbar}\Delta_{\text{corr}}\mathcal{A}^{\epsilon}\right) - 1 \tag{13.152}$$

has the vanishing expectations

$$\begin{aligned}\langle C\rangle_0 &= 0, \\ \langle C\ (\vec{p}\Delta\vec{u})\rangle_0 &= 0,\end{aligned} \tag{13.153}$$

i.e.,

$$\frac{i}{\hbar}\langle\Delta_{\rm corr}\mathcal{A}^\epsilon\rangle_0+\frac{1}{2}\left(\frac{i}{\hbar}\right)^2\langle(\Delta_{\rm corr}\mathcal{A}^\epsilon)^2\rangle_0 = 0, \tag{13.154}$$

$$\frac{i}{\hbar}\langle\Delta_{\rm corr}\mathcal{A}\ (\vec{p}\Delta\vec{u})\rangle_0 = 0, \tag{13.155}$$

as in (13.92), (13.93). In fact, using formula (13.91) the expectation (13.155) is immediately found to be proportional to

$$i\left[-2(2\lambda-1)\frac{D+2}{16}+2(3\lambda-2)\frac{1}{4}+\frac{1}{4}\right], \tag{13.156}$$

which vanishes identically in λ for $D=4$. Similarly, using formula (13.90), the first term in (13.154) has an expectation proportional to

$$i\left[-2\left(\frac{1}{4}-\lambda\right)\frac{(D+2)D}{16}-4\lambda^2\frac{D+2}{16}-(3\lambda-2)\left(\frac{D}{4}-\frac{2}{4}\right)-\left(\frac{D}{4}-\frac{3}{8}\right)\right], \tag{13.157}$$

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

$$-i\frac{3}{8}(2\lambda-1)^2, \tag{13.158}$$

to which the second term adds

$$i\,\frac{1}{2}\left[4(2\lambda-1)^2\frac{(D+4)(D+2)}{64}+9(2\lambda-1)^2\frac{1}{4}-12(2\lambda-1)^2\frac{D+2}{16}\right], \tag{13.159}$$

which cancels (13.159) for $D=4$. Thus the sum of all time slicing corrections vanishes also in the three-dimensional case.

13.6 Geometric Argument for Absence of Time Slicing Corrections

As mentioned before, the basic reason for the absence of the time slicing corrections can be shown to be the property of the connection

$$\Gamma_\mu{}^{\mu\lambda}=g^{\mu\nu}e_i{}^\lambda\partial_\mu e^i{}_\nu=0, \tag{13.160}$$

which, in turn, follows from the basic identity $\partial_\mu e^i_\mu=0$ satisfied by the basis tetrad, and from the diagonality of the metric $g^{\mu\nu}\propto\delta^{\mu\nu}$. Indeed, it is possible to apply the techniques of Sections 10.1, 10.2 to the general pseudotime evolution amplitude (12.28) with the regulating functions

$$f_l=f(\mathbf{x}),\quad f_r\equiv 1. \tag{13.161}$$

Since this regularization affects only the postpoints at each time slice, it is straightforward to repeat the derivation of an equivalent short-time amplitude given in Section 11.3. The result can be expressed in the form (dropping subscripts n)

$$K^\epsilon(\Delta q)=\frac{\sqrt{g(q)}}{\sqrt{2\pi i\epsilon\hbar f/M}^D}\exp\left[\frac{i}{\hbar}(\mathcal{A}^\epsilon+\mathcal{A}^\epsilon_J)\right], \tag{13.162}$$

where f abbreviates the postpoint value $f(\mathbf{x}_n)$ and $\mathcal{A}^\epsilon$ is the short-time action

$$\mathcal{A}^\epsilon=\frac{M}{2\epsilon f}g_{\mu\nu}(q)\Delta q^\mu\Delta q^\nu. \tag{13.163}$$

There exists now a simple expression for the Jacobian action. Using formula (11.75), it becomes simply

$$\frac{i}{\hbar}\mathcal{A}_J^\epsilon = \frac{1}{2}\Gamma_\mu{}^\mu{}_\nu \Delta q^\nu - i\epsilon\frac{\hbar f}{8M}(\Gamma_\mu{}^\mu{}_\nu)^2. \tag{13.164}$$

In the postpoint formulation, the measure needs no further transformation. This can be seen directly from the time-sliced expression (13.8) for $\lambda = 0$ or, more explicitly, from the vanishing of the extra action $\mathcal{A}_f^\epsilon$ in (13.74) for $D = 2$ and in (13.149) for $D = 3$. As a result, the vanishing contracted connection appearing in (13.164) makes *all* time-slicing corrections vanish. Only the basic short-time action (13.163) survives:

$$\Delta\mathcal{A}^\epsilon = 4M\frac{(\Delta\mathbf{u})^2}{2\epsilon_s}. \tag{13.165}$$

Thanks to this fortunate circumstance, the formal solution found in 1979 by Duru and Kleinert happens to be correct.

13.7 Comparison with Schrödinger Theory

For completeness, let us also show the significance of the geometric property $\Gamma_\mu{}^{\mu\lambda} = 0$ within the Schrödinger theory. Consider the Schrödinger equation of the Coulomb system

$$\left(-\frac{1}{2M}\hbar^2\boldsymbol{\nabla}^2 - E\right)\psi(\mathbf{x}) = \frac{e^2}{r}\psi(\mathbf{x}), \tag{13.166}$$

to be transformed to that of a harmonic oscillator. The postpoint regularization of the path integral with the functions (13.161) corresponds to multiplying the Schrödinger equation with $f_l = r$ from the left. This gives

$$\left(-\frac{1}{2M}\hbar^2 r\boldsymbol{\nabla}^2 - Er\right)\psi(\mathbf{x}) = e^2\psi(\mathbf{x}). \tag{13.167}$$

We now go over to the square root coordinates u^μ transforming $-Er$ into the harmonic potential $-E(u^\mu)^2$ and the Laplacian $\boldsymbol{\nabla}^2$ into $g^{\mu\nu}\partial_\mu\partial_\nu - \Gamma_\mu{}^{\mu\lambda}\partial_\lambda$. The geometric property $\Gamma_\mu{}^{\mu\lambda} = 0$ ensures now the absence of the second term and the result is simply $g^{\mu\nu}\partial_\mu\partial_\nu$. Since $g^{\mu\nu} = \delta^{\mu\nu}/4r$, the Schrödinger equation (13.167) takes the simple form

$$\left[-\frac{1}{8M}\hbar^2\partial_\mu^2 - E(u^\mu)^2\right]\psi(u^\mu) = e^2\psi(u^\mu). \tag{13.168}$$

Due to the factor $(u^\mu)^2$ accompanying the energy E, the physical scalar product in which the states of different energies are orthogonal to each other is given by

$$\langle\psi'|\psi\rangle = \int d^4u\psi'(u^\mu)(u^\mu)^2\psi(u). \tag{13.169}$$

This corresponds precisely to the scalar product given in Eq. (11.95) with the purpose of making the Laplace operator (here $\Delta = (1/4\mathbf{u}^2)\partial_{\mathbf{u}}^2$) hermitian in the u^μ-space with torsion. Indeed, the once-contracted torsion tensor $S_\mu = S_{\mu\nu}{}^\nu$ can be written as a gradient of a scalar function:

$$S_\mu = \partial_\mu \sigma(\vec{u}), \quad \sigma(\vec{u}) = \frac{1}{2}\log \vec{u}^2. \tag{13.170}$$

Quite generally, we have shown in Eq. (11.104) that if $S_\mu(q)$ is a partial derivative of a scalar field $\sigma(q)$, the physical scalar product is given by (11.95):

$$\langle \psi_2 | \psi_1 \rangle_{\rm phys} \equiv \int d^D q \sqrt{g(q)} e^{-2\sigma(q)} \psi_2^*(q) \psi_1(q). \tag{13.171}$$

From (13.137), we have

$$\sqrt{g} = 16\vec{u}^4, \tag{13.172}$$

so that the physical scalar product is

$$\langle \psi_2 | \psi_1 \rangle_{\rm phys} = \int d^4 u \sqrt{g} e^{-2\sigma} \psi_2^*(\vec{u}) \psi_1(\vec{u}) = \int d^4 u \, 16\vec{u}^2 \, \psi_2^*(\vec{u}) \psi_1(\vec{u}). \tag{13.173}$$

The Laplace operator obtained from $\partial_{\vec{x}}^2$ by the nonholonomic Kustaanheimo-Stiefel transformation is $\Delta = (1/4\vec{u}^2)\partial_\mu^2$. This is Hermitian in the physical scalar product (13.173), but not in the naive one (11.90) with the integral measure $\int d^4 u \, 16\vec{u}^4$.

In two dimensions, the torsion vanishes and the physical scalar product reduces to the naive one:

$$\langle \psi_2 | \psi_1 \rangle_{\rm phys} = \int d^2 u \sqrt{g} \psi_2^*(\mathbf{u}) \psi_1(\mathbf{u}) = \int d^2 u \, 4\mathbf{u}^2 \psi_2^*(\mathbf{u}) \psi_1(\mathbf{u}). \tag{13.174}$$

With $\mu = 4M$ and $-E = \mu\omega^2/2$, Eq. (13.168) is the Schrödinger equation of a harmonic oscillator:

$$\left[-\frac{1}{2\mu}\hbar^2 \partial_\mu^2 + \frac{\mu}{2}\omega^2 (u^\mu)^2 \right] \psi(u^\mu) = \mathcal{E}\psi(u^\mu). \tag{13.175}$$

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

$$\mathcal{E}_N = \hbar\omega(N + D_u/2), \tag{13.176}$$

where $D_u = 4$ is the dimension of u^μ-space,

$$N = \sum_{i=1}^{D_u} n_i \tag{13.177}$$

sums up the integer principal quantum numbers of the factorized wave functions in each direction of the u^μ-space. The multivaluedness of the mapping from $\mathbf{x}$ to u^μ allows only symmetric wave functions to be associated with Coulomb states. Hence

N must be even and can be written as $N = 2(n-1)$. The pseudoenergy spectrum is therefore

$$\mathcal{E}_n = \hbar\omega\, 2(n + D_u/4 - 1), \quad n = 1, 2, 3, \ldots\ . \tag{13.178}$$

According to (13.175), the Coulomb wave functions must all have a pseudoenergy

$$\mathcal{E}_n = e^2. \tag{13.179}$$

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

$$\omega = \omega_n \equiv \frac{e^2}{2(n + D_u/4 - 1)}, \quad n = 1, 2, 3\ldots\ . \tag{13.180}$$

With $\omega^2 = -E/2M$ and $D_u = 4$, this yields the Coulomb,energies

$$E_n = -2M\omega_n^2 = -\frac{Me^4}{\hbar^2}\frac{1}{2n^2} = -Mc^2\frac{\alpha^2}{2n^2}, \tag{13.181}$$

showing that the number $N/2 = n - 1$ corresponds to the usual principal quantum number of the Coulomb wave functions.

Let us now focus our attention upon the three-dimensional Coulomb system where $D_u = 4$. In this case, not all even oscillator wave functions correspond to Coulomb bound-state wave functions. This follows from the fact that the Coulomb wave functions do not depend on the dummy fourth coordinate x^4 (or the dummy angle γ). Thus they satisfy the constraint $\partial_{x^4}\psi = 0$, implying in u^μ-space [recall (13.137)]

$$\begin{aligned} -ir\partial_{x^4}\psi(\mathbf{x}) &= -ire_4{}^\mu\partial_\mu\psi(u^\mu) = -i\frac{1}{2}\left[(u^2\partial_1 - u^1\partial_2) + (u^4\partial_3 - u^3\partial_4)\right]\psi(u^\mu) \\ &= -i\partial_\gamma\psi(u^\mu) = 0. \end{aligned} \tag{13.182}$$

The explicit construction of the oscillator and Coulomb bound-state wave functions is most conveniently done in terms of the complex coordinates (13.101). In terms of these, the constraint (13.182) reads

$$\frac{1}{2}\left[\bar{z}\partial_{\bar{z}} - z\partial_z\right]\psi(z, z^*) = 0. \tag{13.183}$$

This will be used below to select the Coulomb states.

To solve the Schrödinger equation (13.175) we simplify the notation by going over to *atomic natural units*, where $\hbar = 1, M = 1, e^2 = 1$, $\mu = 4M = 4$. All lengths are measured in units of the Bohr radius (4.376), whose numerical value is $a_H = \hbar^2/Me^2 = 5.2917 \times 10^{-9}$ cm, all energies in units of $E_H \equiv e^2/a_H = Me^4/\hbar^2 = 4.359 \times 10^{-11}$ erg $= 27.210$ eV, and all frequencies ω in units of $\omega_H \equiv$

$Me^4/\hbar^3 = 4.133 \times 10^{16}/\text{sec}(= 4\pi\times$ Rydberg frequency $\nu_R)$. Then (13.175) reads (after multiplication by $4M/\hbar^2$)

$$\hat{h}\psi(u^\mu) \equiv \frac{1}{2}\left[-\partial_\mu^2 + 16\omega^2(u^\mu)^2\right]\psi(u^\mu) = 4\psi(u^\mu). \tag{13.184}$$

The spectrum of the operator $\hat{h}$ is obviously $4\omega(N+2) = 8\omega n$. To satisfy the equation, the frequency ω has to be equal to $\omega_n = 1/2n$.

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

$$\hat{h}^s = \frac{1}{2}\left[-\partial_\mu^2 + 4(u^\mu)^2\right], \tag{13.185}$$

with the help of the ω-dependent transformation

$$\hat{h} = 4\omega e^{i\vartheta\hat{D}}\hat{h}^s e^{-i\vartheta\hat{D}}, \tag{13.186}$$

in which the operator $\hat{D}$ is an infinitesimal *dilation operator* which in this context is called *tilt operator* [12, 13]:

$$\hat{D} \equiv -\frac{1}{2}iu^\mu\partial_\mu, \tag{13.187}$$

and ϑ is the *tilt angle*

$$\vartheta = \log(2\omega). \tag{13.188}$$

The Coulomb wave functions are therefore given by the rescaled solutions of the standardized Schrödinger equation (13.185):

$$\psi(u^\mu) = e^{i\vartheta\hat{D}}\psi^s(u^\mu) = \psi^s(\sqrt{2\omega}u^\mu). \tag{13.189}$$

Note that for a solution with a principal quantum number n the scale parameter $\sqrt{2\omega}$ depends on n:

$$\psi_n(u^\mu) = \psi_n^s(u^\mu/\sqrt{n}). \tag{13.190}$$

The standardized wave functions $\psi_n^s(u^\mu)$ are constructed most conveniently by means of four sets of creation and annihilation operators $\hat{a}_1^\dagger, \hat{a}_2^\dagger, \hat{b}_1^\dagger, \hat{b}_2^\dagger$, and $\hat{a}_1, \hat{a}_2, \hat{b}_1, \hat{b}_2$. They are combinations of z_1, z_2, their complex-conjugates, and the associated differential operators $\partial_{z_1}, \partial_{z_2}, \partial_{z_1^*}, \partial_{z_2^*}$. The combinations are the same as in (9.127), (9.128), written down once for z_1 and once for z_2. In addition, we choose the indices so that a_i and b_i transform by the same spinor representation of the rotation group. If c_{ij} is the 2×2 matrix

$$c = i\sigma^2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{13.191}$$

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

$$\hat{a}_1^\dagger \equiv -\frac{1}{\sqrt{2}}(-\partial_{z_2^*} + z_2), \qquad \hat{b}_1^\dagger \equiv \frac{1}{\sqrt{2}}(-\partial_{z_1} + z_1^*),$$
$$\hat{a}_2^\dagger \equiv \frac{1}{\sqrt{2}}(-\partial_{z_1^*} + z_1), \qquad \hat{b}_2^\dagger \equiv \frac{1}{\sqrt{2}}(-\partial_{z_2} + z_2^*), \tag{13.192}$$

and the annihilation operators

$$\hat{a}_1 \equiv -\frac{1}{\sqrt{2}}(\partial_{z_2} + z_2^*), \qquad \hat{b}_1 \equiv \frac{1}{\sqrt{2}}(\partial_{z_1^*} + z_1),$$
$$\hat{a}_2 \equiv \frac{1}{\sqrt{2}}(\partial_{z_1} + z_1^*), \qquad \hat{b}_2 \equiv \frac{1}{\sqrt{2}}(\partial_{z_2^*} + z_2). \tag{13.193}$$

Note that $\partial_z^\dagger = -\partial_{z^*}$. The standardized oscillator Hamiltonian is then

$$\hat{h}^s = 2(\hat{a}^\dagger\hat{a} + \hat{b}^\dagger\hat{b} + 2), \tag{13.194}$$

where we have used the same spinor notation as in (13.99). The ground state of the four-dimensional oscillator is annihilated by $\hat{a}_1, \hat{a}_2$ and $\hat{b}_1, \hat{b}_2$. It has therefore the wave function

$$\langle z, z^*|0\rangle = \psi_{s,0000}(z, z^*) = \frac{1}{\sqrt{\pi}}e^{-z_1z_1^* - z_2z_2^*} = \frac{1}{\sqrt{\pi}}e^{-(u^\mu)^2}. \tag{13.195}$$

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

$$|n_1^a, n_2^a, n_1^b, n_2^b\rangle = N_{n_1^a,n_2^a,n_1^b,n_2^b}\ \hat{a}_1^{\dagger n_1^a}\hat{a}_2^{\dagger n_2^a}\hat{b}_1^{\dagger n_1^b}\hat{b}_2^{\dagger n_2^b}|0\rangle, \tag{13.196}$$

with the normalization factor

$$N_{n_1^a,n_2^a,n_1^b,n_2^b} = \frac{1}{\sqrt{n_1^a!n_2^a!n_1^b!n_2^b!}}. \tag{13.197}$$

The eigenvalues of $\hat{h}^s$ are obtained from the sum of the number of a- and b-quanta as

$$2(n_1^a + n_2^a + n_1^b + n_2^b + 2) = 2(N + 2) = 4n. \tag{13.198}$$

The Coulomb bound-state wave functions are in one-to-one correspondence with those oscillator wave functions which satisfy the constraint (13.183), which may now be written as

$$\hat{L}_{05} = -\frac{1}{2}(\hat{a}^\dagger\hat{a} - \hat{b}^\dagger\hat{b})\psi^s = 0. \tag{13.199}$$

These states carry an equal number of a- and b-quanta. They diagonalize the (mutually commuting) a- and b-spins

$$\hat{L}_i^a \equiv \frac{1}{2}\hat{a}^\dagger\sigma_i\hat{a}, \quad \hat{L}_i^a \equiv \frac{1}{2}\hat{b}^\dagger\sigma_i\hat{b}, \tag{13.200}$$

with the quantum numbers

$$\begin{aligned} l^a &= (n_1^a + n_2^a)/2, \quad m^a = (n_1^a - n_2^a)/2, \\ l^b &= (n_1^b + n_2^b)/2, \quad m^b = (n_1^b - n_2^b)/2, \end{aligned} \tag{13.201}$$

where l, m are the eigenvalues of $\hat{L}^2$, $\hat{L}_3$. By defining

$$\begin{aligned} n_1^a &\equiv n_1 + m, \quad n_2^a \equiv n_2, \quad n_1^b = n_2 + m, \quad n_2^b = n_1, \qquad \text{for } m \geq 0, \\ n_1^a &\equiv n_1, \quad n_2^a \equiv n_2 - m, \quad n_1^b = n_2, \quad n_2^b = n_1 - m, \qquad \text{for } m \leq 0, \end{aligned} \tag{13.202}$$

we establish contact with the eigenstates $|n_1, n_2, m\rangle$ which arise naturally when diagonalizing the Coulomb Hamiltonian in parabolic coordinates. The relation between these states and the usual Coulomb wave function of a given angular momentum $|nlm\rangle$ is obvious since the angular momentum operator $\hat{L}_i$ is equal to the sum of a- and b-spins. The rediagonalization is achieved by the usual vector coupling coefficients (see the last equation in Appendix 13A).

Note that after the tilt transformation (13.189), the exponential behavior of the oscillator wave functions $\psi_n^s(u^\mu) \propto \text{polynomial}(u^\mu) \times e^{-(u^\mu)^2}$ goes correctly over into the exponential r-dependence of the Coulomb 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 $e^{i\vartheta\hat{D}}$ at a *fixed* angle ϑ is unitary, the Coulomb bound states ψ_n, arising from the complete set of oscillator states ψ_n^s by applying $e^{i\vartheta\hat{D}}$, do *not* span the Hilbert space. Due to the n-dependence of the tilt angle $\vartheta_n = \log(1/n)$, a section of the Hilbert space is not reached. The continuum states of the Coulomb system, which are obtained by tilting another complete set of states, precisely fill this section. Intuitively we can understand this incompleteness simply as follows. The wave functions $\psi_n^s(u^\mu)$ have for increasing n spatial oscillations with shorter and shorter wavelength. These allow the completeness sum $\sum_n \psi_n^s(u^\mu)\psi_n^{s*}(u^\mu)$ to build up a δ-function which is necessary to span the Hilbert space. In contrast, when forming the sum of the dilated wave functions

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

the terms of larger n have increasingly stretched spatial oscillations which are *not* sufficient to build up an infinitely narrow distribution.

A few more algebraic properties of the creation and annihilation operator representation of the Coulomb wave functions are collected in Appendix 13A and 13.10.

13.8 Angular Decomposition of Amplitude, and Radial Wave Functions

Let us also give an angular decomposition of the fixed-energy amplitude. This serves as a convenient starting point for extracting the radial wave functions of the

Coulomb system which will, in Chapter 14, enable us to find the Coulomb amplitude to D dimensions. We begin with the expression (13.133),

$$
\begin{aligned}
(\mathbf{x}_b|\mathbf{x}_a)_E &= -i\frac{M\kappa}{\pi\hbar}\int_0^1 d\varrho\frac{\varrho^{-\nu}}{(1-\varrho)^2}I_0\left(2\kappa\frac{2\sqrt{\varrho}}{1-\varrho}\sqrt{(r_br_a+\mathbf{x}_b\mathbf{x}_a)/2}\right)\\
&\quad\times\exp\left\{-\kappa\frac{1+\varrho}{1-\varrho}(r_b+r_a)\right\}, \qquad (13.203)
\end{aligned}
$$

and rewrite the Bessel function as $I_0(z\cos(\theta/2))$, where θ is the relative angle between $\mathbf{x}_a$ and $\mathbf{x}_b$, and

$$
z \equiv 2\kappa\sqrt{r_br_a}\frac{2\sqrt{\varrho}}{1-\varrho}. \qquad (13.204)
$$

Now we make use of the expansion[1]

$$
\left(\frac{1}{2}kz\right)^{\mu-\nu}I_\nu(kz) = k^\mu\sum_{l=0}^{\infty}\frac{1}{l!}\frac{\Gamma(l+\mu)}{\Gamma(1+\nu)}(2l+\mu)F(-l,l+\mu;1+\nu;k^2)(-)^lI_{2l+\mu}(z). \qquad (13.205)
$$

Setting $k=\cos(\theta/2)$, $\nu=2q>0$, $\mu=1+2q$, and using formulas (1.445), (1.446) for the rotation functions, this becomes

$$
I_{2q}(z\cos(\theta/2)) = \frac{2}{z}\sum_{l=|q|}^{\infty}(2l+1)d^l_{qq}(\theta)I_{2l+1}(z), \qquad (13.206)
$$

reducing for $q=0$ to

$$
I_0(z\cos(\theta/2)) = \frac{2}{z}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)I_{2l+1}(z). \qquad (13.207)
$$

After inserting this into (13.133) and substituting $y=-\frac{1}{2}\log\varrho$, so that

$$
\varrho = e^{-2y}, \qquad z = 2\kappa\sqrt{r_br_a}\frac{1}{\sinh y}, \qquad (13.208)
$$

we expand the fixed-energy amplitude into spherical harmonics

$$
\begin{aligned}
(\mathbf{x}_b|\mathbf{x}_a)_E &= \frac{1}{r_br_a}\sum_{l=0}^{\infty}(r_b|r_a)_{E,l}\frac{2l+1}{4\pi}P_l(\cos\theta)\\
&= \frac{1}{r_br_a}\sum_{l=0}^{\infty}(r_b|r_a)_{E,l}\sum_{m=-l}^{l}Y_{lm}(\hat{\mathbf{x}}_b)Y^*_{lm}(\hat{\mathbf{x}}_a), \qquad (13.209)
\end{aligned}
$$

[1] G.N. Watson, *Theory of Bessel Functions*, Cambridge University Press, London, 1966, 2nd ed., p.140, formula (3).

with the radial amplitude

$$
\begin{aligned}
(r_b|r_a)_{E,l} &= -i\sqrt{r_b r_a}\frac{2M}{\hbar}\int_0^\infty dy \frac{1}{\sinh y} e^{2\nu y} \\
&\quad\times \exp\left[-\kappa \coth y (r_b + r_a)\right] I_{2l+1}\left(2\kappa\sqrt{r_b r_a}\frac{1}{\sinh y}\right).
\end{aligned}
\tag{13.210}
$$

Now we apply the integral formula (9.29) and find

$$
(r_b|r_a)_{E,l} = -i\frac{M}{\hbar\kappa}\frac{\Gamma(-\nu+l+1)}{(2l+1)!} W_{\nu,l+1/2}\left(2\kappa r_b\right) M_{\nu,l+1/2}\left(2\kappa r_a\right). \tag{13.211}
$$

On the right-hand side the energy E is contained in the parameters $\kappa = \sqrt{-2ME/\hbar^2}$ and $\nu = e^2/2\omega\hbar = \sqrt{-e^4M/2\hbar^2 E}$. The Gamma function has poles at $\nu = n$ with $n = l+1, l+2, l+3, \ldots$. These correspond to the bound states of the Coulomb system at the energy eigenvalues

$$
E_n = -\frac{Me^4}{\hbar^2}\frac{1}{2n^2} = -Mc^2\frac{\alpha^2}{2n^2}. \tag{13.212}
$$

Writing

$$
\kappa = \frac{1}{a_H}\frac{1}{\nu}, \tag{13.213}
$$

with the Bohr radius

$$
a_H \equiv \frac{\hbar^2}{Me^2} \tag{13.214}
$$

(for the electron, $a_H \approx 0.529 \times 10^{-8}$cm), we have the approximations near the poles at $\nu \approx n$,

$$
\begin{aligned}
\Gamma(-\nu+l+1) &\approx -\frac{(-)^{n_r}}{n_r!}\frac{1}{\nu-n}, \\
\frac{1}{\nu-n} &\approx \frac{2}{n}\frac{\hbar^2\kappa^2}{2M}\frac{1}{E-E_n}, \\
\kappa &\approx \frac{1}{a_H}\frac{1}{n},
\end{aligned}
\tag{13.215}
$$

where $n_r = n - l - 1$. Hence

$$
-i\Gamma(-\nu+l+1)\frac{M}{\hbar\kappa} \approx \frac{(-)^{n_r}}{n^2 n_r!}\frac{1}{a_H}\frac{i\hbar}{E-E_n}. \tag{13.216}
$$

Let us expand the pole parts of the spectral representation of the radial fixed-energy amplitude in the form

$$
(r_b|r_a)_{E,l} = \sum_{n=l+1}^{\infty}\frac{i\hbar}{E-E_n}R_{nl}(r_b)R_{nl}(r_a) + \ldots\ . \tag{13.217}
$$

The radial wave functions defined by this expansion correspond to the normalized bound-state wave functions

$$\psi_{nlm}(\mathbf{x}) = \frac{1}{r} R_{n,l}(r) Y_{lm}(\hat{\mathbf{x}}). \tag{13.218}$$

By comparing the pole terms of (13.211) and (13.217) [using (13.216) and formula (9.48) for the Whittaker functions, together with (9.50)], we identify the radial wave functions as

$$\begin{aligned} R_{nl}(r) &= \frac{1}{a_H^{1/2} n} \frac{1}{(2l+1)!} \sqrt{\frac{(n+l)!}{(n-l-1)!}} \\ &\times (2r/na_H)^{l+1} e^{-r/na_H} M(-n+l+1, 2l+2, 2r/na_H) \\ &= \frac{1}{a_H^{1/2} n} \sqrt{\frac{(n-l-1)!}{(n+l)!}} e^{-r/na_H} (2r/na_H)^{l+1} L_{n-l-1}^{2l+1}(2r/na_H). \end{aligned} \tag{13.219}$$

To obtain the last expression we have used formula (9.53).[2] It must be noted that the normalization integrals of the wave functions $R_{nl}(r)$ differ by a factor $z/2n = (2r/na_H)/2n$ from those of the harmonic oscillator (9.54), which are contained in integral tables. However, due to the recursion relation for the Laguerre polynomials

$$zL_n^\mu(z) = (2n+\mu+1)L_n^\mu(z) - (n+\mu)L_{n-1}^\mu(z) - (n+1)L_{n+1}^\mu(z), \tag{13.220}$$

the factor $z/2n$ leaves the values of the normalization integrals unchanged. The orthogonality of the wave functions with different n is much harder to verify since the two Laguerre polynomials in the integrals have different arguments. Here the group-theoretic treatment of Appendix 13A provides the simplest solution. The orthogonality is shown in Eq. (13A.28).

We now turn to the continuous wave functions. The fixed-energy amplitude has a cut in the energy plane for positive energy where $\kappa = -ik$ and $\nu = i/a_H k$ are imaginary. In this case we write $\nu = i\nu'$. From the discontinuity we can extract the scattering wave functions. The discontinuity is given by

$$\begin{aligned} \text{disc}\,(r_b|r_a)_{E,l} &= (r_b|r_a)_{E+i\eta,l} - (r_b|r_a)_{E-i\eta,l} \\ &= \frac{M}{\hbar k}\left[\frac{\Gamma(-i\nu'+l+1)}{(2l+1)!} W_{i\nu',l+1/2}(-2ikr_b)\, M_{i\nu',l+1/2}(-2ikr_a) + (\nu' \to -\nu')\right]. \end{aligned} \tag{13.221}$$

In the second term, we replace

$$M_{i\nu',l+1/2}(-2ikr) = e^{-i\pi(l+1)} M_{-i\nu',l+1/2}(2ikr), \tag{13.222}$$

and use the relation, valid for $\arg z \in (-\pi/2, 3\pi/2)$, $2\mu \neq -1, -2, -3, \dots$,

$$M_{\lambda,\mu}(z) = \frac{\Gamma(2\mu+1)}{\Gamma(\mu+\lambda+1/2)} e^{i\pi\lambda} e^{-i\pi(\mu+1/2)} W_{\lambda,\mu}(z) + \frac{\Gamma(2\mu+1)}{\Gamma(\mu-\lambda+1/2)} e^{i\pi\lambda} W_{-\lambda,\mu}(e^{i\pi}z), \tag{13.223}$$

[2] Compare L.D. Landau and E.M. Lifshitz, *Quantum Mechanics*, Pergamon, London, 1965, p. 119. Note the different definition of our Laguerre polynomials $L_n^\mu = [(-)^\mu/(n+\mu)!] L_{n+\mu}{}^\mu|_{\text{L.L.}}$.

to find

$$\mathrm{disc}\,(r_b|r_a)_{E,l} = \frac{M}{\hbar k}\frac{|\Gamma(-i\nu'+l+1)|^2}{(2l+1)!^2}e^{\pi\nu'}M_{i\nu',l+1/2}\,(-2ikr_b)\,M_{-i\nu',l+1/2}\,(2ikr_a)\,. \tag{13.224}$$

The continuum states enter the completeness relation as

$$\int_0^\infty \frac{dE}{2\pi\hbar}\mathrm{disc}\,(r_b|r_a)_{E,l} + \sum_{n=l+1}^{\infty} R_{nl}(r_b)R^*_{nl}(r_a) = \delta(r_b - r_a) \tag{13.225}$$

[compare (1.330)]. Inserting (13.221) and replacing the continuum integral $\int_0^\infty dE/2\pi\hbar$ by the momentum integral $\int_{-\infty}^\infty dk k\hbar/2\pi M$, the continuum part of the completeness relation becomes

$$\int_{-\infty}^{\infty} dk R_{kl}(r_b)R^*_{kl}(r_a), \tag{13.226}$$

with the radial wave functions

$$R_{kl}(r) = \sqrt{\frac{1}{2\pi}}\frac{|\Gamma(-i\nu'+l+1)|}{(2l+1)!}e^{\pi\nu'/2}M_{i\nu',l+1/2}(-2ikr). \tag{13.227}$$

By expressing the Whittaker function $M_{\lambda,\mu}(z)$ in terms of the confluent hypergeometric functions, the Kummer functions $M(a,b,z)$, as

$$M_{\lambda,\mu}(z) = z^{\mu+1/2}e^{-z/2}M(\mu-\lambda+1/2, 2\mu+1, z), \tag{13.228}$$

we recover the well-known result of Schrödinger quantum mechanics:[3]

$$R_{kl}(r) = \sqrt{\frac{1}{2\pi}}\frac{|\Gamma(-i\nu'+l+1)|}{(2l+1)!}e^{\pi\nu'/2}e^{ikr}(-2ikr)^{l+1}M(-i\nu'+l+1, 2l+2, -2ikr). \tag{13.229}$$

13.9 Remarks on Geometry of Four-Dimensional u^μ-Space

A few remarks are in order on the Riemann geometry of the $\vec{u}$-space in four dimensions with the metric $g_{\mu\nu} = 4\vec{u}^2\delta_{\mu\nu}$. As in two dimensions, the Cartan curvature tensor $R_{\mu\nu\lambda}{}^\kappa$ vanishes trivially since $e^i{}_\mu(\vec{u})$ is linear in $\vec{u}$:

$$(\partial_\mu\partial_\nu - \partial_\nu\partial_\mu)e^i{}_\lambda(\vec{u}) = 0. \tag{13.230}$$

In contrast to two dimensions, however, the Riemann curvature tensor $\bar{R}_{\mu\nu\lambda}{}^\kappa$ is nonzero. The associated Ricci tensor [see (10.41)], has the matrix elements

$$\begin{aligned}\bar{R}_{\nu\lambda} &= \bar{R}_{\mu\nu\lambda}{}^\mu \\ &= -\frac{3}{2\vec{u}^6}(\delta_{\nu\lambda}\vec{u}^2 - \vec{u}_\nu\vec{u}_\lambda),\end{aligned} \tag{13.231}$$

[3] L.D. Landau and E.M. Lifshitz, op. cit., p. 120.

yielding the scalar curvature

$$\bar{R} = g^{\nu\lambda}\bar{R}_{\nu\lambda} = -\frac{9}{2\vec{u}^4}. \tag{13.232}$$

In general, a diagonal metric of the form

$$g_{\mu\nu}(q) = \Omega^2(q)\delta_{\mu\nu} \tag{13.233}$$

is called *conformally flat* since it can be obtained from a flat space with a unit metric $g_{\mu\nu} = \delta_{\mu\nu}$ by a *conformal transformation* a la Weyl

$$g_{\mu\nu}(q) \to \Omega^2(q) g_{\mu\nu}(q). \tag{13.234}$$

Under such a transformation, the Christoffel symbol changes as follows:

$$\bar{\Gamma}_{\mu\nu}{}^{\lambda} \to \bar{\Gamma}_{\mu\nu}{}^{\lambda} + \Omega_{,\mu}\delta_{\nu}{}^{\lambda} + \Omega_{,\nu}\delta_{\mu}{}^{\lambda} - g_{\mu\nu}g^{\lambda\kappa}\Omega_{,\kappa}, \tag{13.235}$$

the subscript separated by a comma indicating a differentiation, i.e., $\Omega_{,\mu} \equiv \partial_\mu \Omega$.

In D dimensions, the Ricci tensor changes according to

$$\begin{aligned} \bar{R}_{\mu\nu} \;\; &\to \;\; \Omega^{-2}\bar{R}_{\mu\nu} - (D-2)(\Omega^{-3}\Omega_{;\mu\nu} - 2\Omega^{-4}\Omega_{,\mu}\Omega_{,\nu}) \\ &\quad\;\; -g_{\mu\nu}g^{\lambda\kappa}\left[(D-3)\Omega^{-4}\Omega_{,\lambda}\Omega_{,\kappa} + \Omega^{-3}\Omega_{;\lambda\kappa}\right] \\ &= \;\; \Omega^{-2}\bar{R}_{\mu\nu} + (D-2)\Omega^{-1}(\Omega^{-1})_{;\mu\nu} - g_{\mu\nu}(D-2)^{-1}\Omega^{-D}(\Omega^{D-2})_{;\lambda\kappa}g^{\lambda\kappa}. \end{aligned} \tag{13.236}$$

A subscript separated by a semicolon denotes the covariant derivative formed with Riemann connection, i.e.,

$$\Omega_{;\mu\nu} = D_\nu \Omega_{,\mu} = \Omega_{\mu\nu} - \bar{\Gamma}_{\mu\nu}{}^{\lambda}\Omega_{,\lambda}. \tag{13.237}$$

The curvature scalar goes over into

$$\bar{R} \to \bar{R}^{\Omega} = \Omega^{-2}\left[\bar{R} - 2(D-1)\Omega^{-1}\Omega_{;\mu\nu}g^{\mu\nu} - (D-1)(D-4)\Omega^{-2}\Omega_{,\mu}\Omega_{,\nu}g^{\mu\nu}\right]. \tag{13.238}$$

The metric $g_{\mu\nu} = 4\vec{u}^2\delta_{\mu\nu}$ in the $\vec{u}$-space description of the hydrogen atom is conformally flat, so that we can use the above relations to obtain all geometric quantities from the initially trivial metric $g_{\mu\nu} = \delta_{\mu\nu}$ with $\bar{R}_{\mu\nu} = 0$ by inserting $\Omega = 2|\vec{u}|$, so that

$$\Omega_{,\mu} = 2\frac{u^\mu}{|\vec{u}|}, \qquad \Omega_{,\mu\nu} = \frac{2}{|\vec{u}|^3}(\delta^{\mu\nu}\vec{u}^2 - u^\mu u^\nu). \tag{13.239}$$

From the right-hand sides of (13.236) and (13.238) we obtain

$$\begin{aligned} \bar{R}_{\mu\nu} &= -3(D-2)\frac{1}{4\vec{u}^6}(\delta_{\mu\nu}\vec{u}^2 - \vec{u}_\mu\vec{u}_\nu), \\ \bar{R} &= -3(D-1)(D-2)\frac{1}{4\vec{u}^4}. \end{aligned} \tag{13.240}$$

For $D = 4$, these agree with (13.231) and (13.232). For $D = 2$, they vanish.

In the Coulomb system, the conformally flat metric (13.234) arose from the nonholonomic coordinate transformation (13.106) with the basis tetrads (13.137) and their inverses (13.138), which produced the torsion tensor (13.142). In the notation (13.234), the torsion tensor has a contraction

$$S_\mu(q) \equiv S_{\mu\nu^\lambda}(q) = \frac{1}{2\Omega^2(q)}\partial_\mu \Omega^2(q). \tag{13.241}$$

Note that although $S_\mu(q)$ is the gradient of a scalar field, the torsion tensor (13.142) is not a so-called *gradient torsion*, which is defined by the general form

$$S_{\mu\nu}{}^\lambda(q) = \frac{1}{2}\left[\delta_\mu{}^\lambda \partial_\nu s(q) - \delta_\nu{}^\lambda \partial_\mu s(q)\right]. \tag{13.242}$$

For a gradient torsion, $S_\mu(q)$ is also a gradient: $S_\mu(q) = \partial_\mu \sigma(q)$ where $\sigma(q) = (D-1)s(q)/2$. But it is, of course, not the only tensor, for which $S_\mu(q)$ is a gradient.

Note that under a conformal transformation a la Weyl, a massless scalar field $\phi(q)$ is transformed as

$$\phi(q) \to \Omega^{1-D/2}(q)\phi(q). \tag{13.243}$$

The Laplace-Beltrami differential operator $\Delta = \bar{D}^2$ applied to $\phi(q)$ goes over into $\Omega^{1-D/2}(q)\Delta^\Omega \phi(q)$ where

$$\Delta^\Omega = \Omega^{-2}\left[\Delta - \frac{1}{2}(D-2)\Omega^{-1}\Omega_{;\mu\nu}g^{\mu\nu} - \frac{1}{4}(D-2)(D-4)\Omega^{-2}\Omega_{,\mu}\Omega_{,\nu}g^{\mu\nu}\right]. \tag{13.244}$$

Comparison with (13.240) shows that there exists a combination of $\Delta = \bar{D}^2$ and the Riemann curvature scalar $\bar{R}$ which may be called *Weyl-covariant Laplacian*. This combination is

$$\Delta - \frac{1}{4}\frac{D-2}{D-1}\bar{R}. \tag{13.245}$$

When applied to the scalar field it transforms as

$$\left(\Delta - \frac{1}{4}\frac{D-2}{D-1}\bar{R}\right)\phi(q) \longrightarrow \Omega^{-1-D/2}\left(\Delta - \frac{1}{4}\frac{D-2}{D-1}\bar{R}\right)\phi(q). \tag{13.246}$$

Thus we can define a massless scalar field in a conformally invariant way by requiring the vanishing of (13.246) as a wave equation. This symmetry property has made the combination (13.245) a favorite Laplacian operator in curved spaces [14].

13.10 Runge-Lenz-Pauli Group of Degeneracy

A well-known symmetry of the Kepler problem was used by Pauli to find the spectrum of the Coulomb problem by purely algebraic manipulations. There exists a vector operator $\hat{\mathbf{M}}$ constructed from the Hamilton operator $\hat{H}$ of (13.1), the momentum operator $\mathbf{p}$, the angular momentum operator $\hat{\mathbf{L}} \equiv \mathbf{x} \times \hat{\mathbf{p}}$, and the operator $\hat{p}_E \equiv \sqrt{-2M\hat{H}}$. This is the *Runge-Lenz-Pauli vector*:

$$\hat{\mathbf{M}} = \frac{M}{\hat{p}_E}\left[\frac{1}{2M}(\hat{\mathbf{p}} \times \hat{\mathbf{L}} - \hat{\mathbf{L}} \times \hat{\mathbf{p}}) - e^2\frac{\mathbf{r}}{r}\right], \tag{13.247}$$

which commutes with $\hat{H}$ and is therefore a conserved quantity. Together with $\hat{\mathbf{L}}$ it forms the algebra of rotations O(4) in a four-dimensional space

$$[\hat{L}_i, \hat{L}_j] = i\epsilon_{ijk}\hat{L}_k, \quad [\hat{L}_i, \hat{M}_j] = i\epsilon_{ijk}\hat{M}_k, \quad [\hat{M}_i, \hat{M}_j] = i\epsilon_{ijk}\hat{M}_k. \tag{13.248}$$

The vector $\hat{\mathbf{M}}$ is orthogonal to $\hat{\mathbf{L}}$,

$$\hat{\mathbf{M}} \cdot \hat{\mathbf{L}} = \hat{\mathbf{L}} \cdot \hat{\mathbf{M}} = 0, \tag{13.249}$$

and satisfies

$$\hat{\mathbf{L}}^2 + \hat{\mathbf{M}}^2 + \hbar^2 = -e^4 \frac{M}{2\hat{H}} = e^4 \frac{M^2}{\hat{p}_E^2}. \tag{13.250}$$

The combinations

$$\hat{\mathbf{J}}^{(1,2)} \equiv \frac{1}{2}(\hat{\mathbf{L}} \pm \hat{\mathbf{M}}) \tag{13.251}$$

generate commuting Lie algebras of three-dimensional rotations O(3), so that the squares $\left(\hat{\mathbf{J}}^{(1,2)}\right)^2$ have the eigenvalues $j^{(1,2)}(j^{(1,2)}+1)$. The condition (13.249) implies that $j^{(1)} = j^{(2)} = j$. Hence (13.250) becomes

$$\hat{\mathbf{L}}^2 + \hat{\mathbf{M}}^2 + \hbar^2 = 4(\hat{\mathbf{L}} \pm \hat{\mathbf{M}})^2 + \hbar^2 = [4j(j+1)+1]\hbar^2 = e^4 \frac{M^2}{\hat{p}_E^2} = -\hbar^2\alpha^2 \frac{Mc^2}{2\hat{H}}. \tag{13.252}$$

From this follows that $\hat{p}_E$ has the eigenvalues $(2j+1)\alpha Mc$, and $\hat{H}$ the eigenvalues $E_j = -Mc^2\alpha^2/(2j+1)^2$. Thus we identify the principal quantum number as $n = 2j+1 = 0, 1, 2, \dots$. For each n, the magnetic quantum numbers m_1 and m_2 of $\hat{\mathbf{J}}^{(1)}$ and $\hat{\mathbf{J}}^{(2)}$ can run from $-j$ to j, so that each level is $(2j+1)^2 = n^2$-times degenerate.

The wave functions of the hydrogen atom of principal quantum number n are direct products of eigenstates of $\hat{\mathbf{J}}^{(1)}$ and $\hat{\mathbf{J}}^{(2)}$:

$$|n\, m_1 m_2\rangle = |j m_1\rangle^{(1)} \otimes |j m_2\rangle^{(2)}. \tag{13.253}$$

In atomic physics, one prefers combinations of these which diagonalize the orbital angular momentum $\hat{\mathbf{L}} = \hat{\mathbf{J}}^{(1)} + \hat{\mathbf{J}}^{(2)}$. This done with the help of the Clebsch-Gordan coefficients $(j, m_1; j, m_2|l, m)$ [18] which couple spin j with spin j to spin $l = 0, 1, \dots 2j$:

$$|n\, lm\rangle = \sum_{m_1, m_2 = -j,\dots,j} |j m_1\rangle^{(1)} \otimes |j m_2\rangle^{(2)} \, (j, m_1; j, m_2|l, m). \tag{13.254}$$

13.11 Solution in Momentum Space

The path integral for a point particle in a Coulomb potential can also be solved in momentum space.

13.11.1 Pseudotime Path Integral

As in the coordinate space treatment in Section 13.1, we shall calculate the matrix elements of the pseudotime displacement amplitude associated with the the resolvent operator $\hat{R} \equiv i/(E - \hat{H})$. As in Eq. (12.19), we shall rewrite it in the form

$$\hat{R} = \frac{i}{\hat{f}(E - \hat{H})}\hat{f} \tag{13.255}$$

where f is an arbitrary function of space, momentum. Rewriting the the path integral (12.31) in the momentum space representation (2.34), we shall evaluate the canonical path integral for the pseudotime displacement amplitude with $M = 1$:

$$\begin{aligned} \langle \mathbf{p}_b | \hat{\mathcal{U}}_E(S) | \mathbf{p}_a \rangle &= \int \mathcal{D}^3 x(s) \int \frac{\mathcal{D}^3 p(s)}{2\pi\hbar} \\ &\times \exp\left\{ i \int_0^S ds \left[-\mathbf{p}' \cdot \mathbf{x} - f\left(\frac{\mathbf{p}^2}{2} - E\right) + f\,\frac{\alpha}{r} \right] \right\} f_a. \end{aligned} \tag{13.256}$$

From this we find the fixed-energy amplitude via the integral [compare (13.4)]

$$(\mathbf{p}_b | \mathbf{p}_a)_E^f = \int_0^\infty dS \, \langle \mathbf{p}_b | \hat{\mathcal{U}}_E(S) | \mathbf{p}_a \rangle. \tag{13.257}$$

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 [17] of (13.257) under $f \to f'$. Such an invariance permits us to subject (13.257) 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 (13.257) as a path integral

$$(\mathbf{p}_b | \mathbf{p}_a)_E = \int \mathcal{D}f \, \Phi[f] \, (\mathbf{p}_b | \mathbf{p}_a)_E^f. \tag{13.258}$$

The only condition on $\Phi[f]$ is that it must be normalized to have a unit integral: $\int \mathcal{D}f \, \Phi[f] = 1$. The choice which leads to the desired solution of the path integral is

$$\Phi[f] = \prod_s \frac{1}{r} \exp\left\{ -\frac{i}{2r^2} \left[f - r^2 \left(\frac{\mathbf{p}^2}{2} - E \right) \right]^2 \right\}. \tag{13.259}$$

With this, the total action in the path integral (13.258) becomes

$$\mathcal{A}[\mathbf{p}, \mathbf{x}, f] = \int_0^S ds \left[-\mathbf{p}' \cdot \mathbf{x} - \frac{r^2}{2}\left(\frac{\mathbf{p}^2}{2} - E \right)^2 - \frac{1}{2r^2} f^2 + \frac{f}{r}\alpha \right]. \tag{13.260}$$

The path integrals over f and $\mathbf{x}$ in (13.258) are Gaussian and can be done, in this order, yielding a new action

$$\mathcal{A}[\mathbf{p}] = \frac{1}{2} \int_0^S ds \left[\frac{4\mathbf{p}'^2}{\left(\mathbf{p}^2 + p_E^2\right)^2} + \alpha^2 \right], \tag{13.261}$$

where we have introduced $p_E \equiv \sqrt{-2E}$, assuming E to be negative. The positive regime can later be obtained by analytic continuation.

At this point we go to a more symmetric coordinate system in momentum space by projecting the three-vectors $\mathbf{p}$ stereographically to the four-dimensional unit vectors $\vec{\pi} \equiv (\boldsymbol{\pi}, \pi_4)$:

$$\boldsymbol{\pi} \equiv \frac{2p_E\mathbf{p}}{\mathbf{p}^2 + p_E^2}, \qquad \pi_4 \equiv \frac{\mathbf{p}^2 - p_E^2}{\mathbf{p}^2 + p_E^2}. \tag{13.262}$$

This brings (13.261) to the form

$$\mathcal{A}[\vec{\pi}] = \frac{1}{2}\int_0^S ds \left(\frac{1}{p_E^2}\vec{\pi}'^2 + \alpha^2\right). \tag{13.263}$$

The vector $\vec{\pi}$ describes a point particle with pseudomass $\mu = 1/p_E^2$ moving on a four-dimensional unit sphere. The pseudotime evolution amplitude of this system is

$$(\vec{\pi}_b S|\vec{\pi}_a 0) = \int \frac{\mathcal{D}\vec{\pi}}{(2\pi)^{3/2}p_E^3}\, e^{i\mathcal{A}[\vec{\pi}]}. \tag{13.264}$$

Let us see how the measure arises. When integrating out the spatial fluctuations in going from (13.260) to (13.261), the canonical measure in each time slice $[d^3p_n/(2\pi)^3]d^3x_n$ becomes $[d^3p_n/(2\pi)^3][(2\pi)^{1/2}/(\mathbf{p}_n^2 + p_E^2)]^3$. From the stereographic projection (13.262) we see that this is equal to $d\vec{\pi}_n/(2\pi)^{3/2}p_E^3$, where $d\vec{\pi}_n$ denotes the product of integrals over the solid angle on the surface of the unit sphere in four dimensions. The integral $\int d\vec{\pi}$ yields the total surface $2\pi^2$. Alternatively we may rewrite as in Eq. (1.560), $\int d\vec{\pi}_n = \int d^4\pi_n \delta(|\vec{\pi}_n| - 1) = 2\int d^4\pi_n\delta(\vec{\pi}_n^2 - 1)$, or use an explicit angular form of the type (8.120) or (8.124).

The expression (13.264) was obtained by purely formal manipulations on the continuum pseudotime axis and needs, therefore, pseudotime-slicing corrections similar to Section 13.5. For the motion on a spherical surface these have to be evaluated by the methods of Chapter 10. There we learned that the proper sliced path integral we know that in a curved space, the time-sliced measure of path integration is given by the product of invariant integrals $\int dq_n\sqrt{g(q_n)}$ at each time slice, multiplied by an effective action contribution $\exp(i\mathcal{A}_{\rm eff}^\epsilon(q_n)) = \exp(i\epsilon\bar{R}(q_n)/6\mu)$, where $\bar{R}$ is the scalar curvature. For a sphere of radius r in D dimensions, $\bar{R} = (D-1)(D-2)/r^2$, implying here for $D = 4$ that $\exp(i\mathcal{A}_{\rm eff}^\epsilon) = \exp(i\epsilon/\mu) = \exp(i\epsilon\, p_E^2)$. Thus, when transforming the time-sliced measure in the path integral (13.256) to the time-sliced measure on the sphere in (13.264), a factor $e^{iS\,p_E^2}$ is by definition contained in the measure of the path integral (13.264) [compare (10.153), (10.154)]. This has to be compensated by a prefactor $e^{-iS\,p_E^2}$. A careful calculation of the time slicing corrections gives an additional factor $e^{iS\,p_E^2/2}$. The correct version of (13.264) is therefore

$$(\vec{\pi}_b S|\vec{\pi}_a 0) = e^{-iS\,p_E^2/2}\int \frac{\mathcal{D}\vec{\pi}}{(2\pi)^{3/2}p_E^3}\, e^{i\mathcal{A}[\vec{\pi}]}, \tag{13.265}$$

with the integral measure defined as in Eqs. (10.153) and (10.154).

The path integral for the motion near the surface of a sphere in four dimensions was solved Subsection 8.7. The energies were brought on the sphere in Section 8.9. The spectral representation was given explicitly in Eq. (8.162) in terms of rotation matrices. Here we shall use the ultra-pherical harmonics $Y_{lm_1m_2}(\vec{\pi})$ defined in Eq. (8.125). From these we construct combinations appropriate for the hydrogen atom to be denoted by $Y_{n,l,m}(\vec{\pi})$, where n, l, m are the quantum numbers of the hydrogen atom with the well-known ranges ($n = 1, 2, 3, \dots,\ l = 0, \dots, n-1,\ m = -l, \dots, l$). Explictly, these combinations are formed with the help of Clebsch-Gordan coefficients $(j, m_1; j, m_2|l, m)$ [18] which couple spin j with spin j to spin $l = 0, 1, \dots 2j$, where j is related to the principal quantum number by $n = 2j + 1$ [compare (13.254)]:

$$Y_{nlm}(\vec{\pi}) = \sum_{m_1,m_2=-j,\dots,j} Y_{2j,m_1,m_2}(\vec{\pi})\,(j, m_1; j, m_2|l, m)\,. \tag{13.266}$$

The orthonormality and completeness relations are

$$\int d\vec{\pi}\, Y^*_{n'l'm'}(\vec{\pi})Y_{nlm}(\vec{\pi}) = \delta_{nn'}\delta_{ll'}\delta_{mm'}, \quad \sum_{n,l,m} Y_{nlm}(\vec{\pi}')Y_{nlm}(\vec{\pi}) = \delta^{(4)}(\vec{\pi}' - \vec{\pi}), \tag{13.267}$$

where the δ-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:

$$\sum_{l,m} Y_{nlm}(\vec{\pi}')Y_{nlm}(\vec{\pi}) = \frac{n^2}{2\pi^2}P_n(\cos\vartheta), \qquad P_n(\cos\vartheta) = \frac{\sin n\vartheta}{n\sin\vartheta}, \tag{13.268}$$

where ϑ is the angle between the four-vectors $\vec{\pi}_b$ and $\vec{\pi}_a$:

$$\cos\vartheta = \vec{\pi}_b\vec{\pi}_a = \frac{(\mathbf{p}_b^2 - p_E^2)(\mathbf{p}_a^2 - p_E^2) + 4p_E^2\mathbf{p}_b\cdot\mathbf{p}_a}{(\mathbf{p}_b^2 + p_E^2)(\mathbf{p}_a^2 + p_E^2)}. \tag{13.269}$$

Adapting the solution of the path integral for a particle on the surface of a sphere in Eqs. (8.162) with the energy correction of Section 10.4 to the present case we obtain for the path integral in Eq. (13.265) the spectral representation

$$(\vec{\pi}_b S|\vec{\pi}_a 0) = (2\pi)^{3/2}p_E^3 \sum_{n=1}^{\infty} \frac{n^2}{2\pi^2}P_n(\cos\vartheta)\, \exp\left\{\left[-i(p_E^2 n^2 - \alpha^2)\right]\frac{S}{2}\right\}. \tag{13.270}$$

For the path integral in (13.265) itself, the exponential contains the eigenvalues of the squared angular-momentum operator $\hat{L}^2/2\mu$ which in D dimensions are $l(l + D - 2)/2\mu,\quad l = 0, 1, 2, \dots$. For the particle on a sphere in four dimensions and with the identification $l = 2j = n - 1$, the eigenvalues of $\hat{L}^2$ are $n^2 - 1$, leading to an exponential $e^{-i[p_E^2(n^2-1)-\alpha^2]S/2}$. Together with the exponential prefactor in (13.265), we obtain the exponential in (13.270).

Inserting the spectral representation (13.270) into (13.257), we can immediately perform the integral over S, and arrive at the amplitude at zero fixed pseudoenergy

$$(\vec{\pi}_b|\vec{\pi}_a)_0 \quad = \quad (2\pi)^{3/2} p_E^3 \sum_{n=1}^{\infty} \frac{n^2}{2\pi^2} P_n(\cos\vartheta) \, \frac{2i}{2En^2+\alpha^2}. \tag{13.271}$$

This has poles displaying the hydrogen spectrum at energies:

$$E_n = -\frac{\alpha^2}{2n^2}, \quad n = 1, 2, 3, \ldots \,. \tag{13.272}$$

More details on the wave functions are listed in Appendix 13B.

The solution in momentum space was first given by Schwinger [**?**, 20, 21].

13.11.2 Another Form of Action

Consider the following generalization of the action (13.261) containing an arbitrary function h depending on $\mathbf{p}$ and s:

$$\mathcal{A}[\mathbf{p}] = \frac{1}{2} \int_0^S ds \left[\frac{1}{h} \frac{4\mathbf{p}'^2}{(\mathbf{p}^2 + p_E^2)^2} + \alpha^2 h \right]. \tag{13.273}$$

This action is invariant under reparametrizations $s \to s'$ if one transforms simultaneously $h \to h ds/ds'$. The path integral with the action (13.261) in the exponent may thus be viewed as a path integral with the gauge-invariant action (13.273) and an additional path integral $\int df \, \Phi[f]$ with an arbitrary gauge-fixing functional $\Phi[h]$. The parameter s may be chosen to be the physical time t. By going to the extremum in h, the action reduces to

$$\mathcal{A}[\mathbf{p}] = 2\alpha \int_{\tau_a}^{\tau_b} d\tau \sqrt{\frac{\dot{\mathbf{p}}^2}{(\mathbf{p}^2 + p_E^2)^2}}. \tag{13.274}$$

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

$$S(\mathbf{p}_b, \mathbf{p}_a; E) = -\int_{\mathbf{p}_a}^{\mathbf{p}_b} d\tau \, \dot{\mathbf{p}} \cdot \mathbf{x}. \tag{13.275}$$

The eikonal (13.275), and thus the action (13.274), determines the classical orbits via the first extremal principle of theoretical mechanics found in 1744 by Maupertius (see p. 380 and [22]).

Appendix 13A Dynamical Group of Coulomb States

The subspace of oscillator wave functions $\psi^s(u^\mu/\sqrt{n})$ in the standardized form (13.189), which do not depend on x^4 (i.e., on γ), is obtained by applying an equal number of creation operators $a^\dagger$

and $b^\dagger$ to the ground state wave function (13.195). They are equal to the scalar products between the localized bra states $\langle z, z^*|$ and the ket states $|n_1^a, n_2^a, n_1^b, n_2^b\rangle$ of (13.196).

These ket states form an irreducible representation of the dynamical group O(4,2), the orthogonal group of six-dimensional flat space whose metric g_{AB} has four positive and two negative entries $(1,1,1,1,-1,-1)$.

The 15 generators $\hat{L}_{AB} \equiv -\hat{L}_{BA},\ \ A,B = 1,\dots 6$, of this group are constructed from the spinors

$$\hat{a} \equiv \begin{pmatrix} \hat{a}_1 \\ \hat{a}_2 \end{pmatrix}, \quad \hat{b} \equiv \begin{pmatrix} \hat{b}_1 \\ \hat{b}_2 \end{pmatrix}, \tag{13A.1}$$

and their Hermitian-adjoints, using the Pauli σ-matrices and $c \equiv i\sigma^2$, as follows (since L_{ij} carry subscripts, we define $\sigma_i \equiv \sigma^i$):

$$\begin{aligned}
\hat{L}_{ij} &= \tfrac{1}{2}\left(\hat{a}^\dagger\sigma_k\hat{a} + \hat{b}^\dagger\sigma_k\hat{b}\right) \quad i,j,k = 1,2,3 \text{ cyclic},\\
\hat{L}_{i4} &= \tfrac{1}{2}\left(\hat{a}^\dagger\sigma_i\hat{a} - \hat{b}^\dagger\sigma_i\hat{b}\right),\\
\hat{L}_{i5} &= \tfrac{1}{2}\left(\hat{a}^\dagger\sigma_i c\hat{b}^\dagger - \hat{a}c\sigma_i\hat{b}\right),\\
\hat{L}_{i6} &= \tfrac{i}{2}\left(\hat{a}^\dagger\sigma_i c\hat{b}^\dagger + \hat{a}c\sigma_i\hat{b}\right),\\
\hat{L}_{45} &= \tfrac{1}{2i}\left(\hat{a}^\dagger c\hat{b}^\dagger - \hat{a}c\hat{b}\right),\\
\hat{L}_{46} &= \tfrac{1}{2}\left(\hat{a}^\dagger c\hat{b}^\dagger + \hat{a}c\hat{b}\right),\\
\hat{L}_{56} &= \tfrac{1}{2}\left(\hat{a}^\dagger\hat{a} + \hat{b}^\dagger\hat{b} + 2\right).
\end{aligned} \tag{13A.2}$$

The eigenvalues of $\hat{L}_{56}$ on the states with an equal number of a- and b-quanta are obviously

$$\frac{1}{2}\left(n_1^a + n_2^a + n_1^b + n_2^b + 2\right) = n. \tag{13A.3}$$

The commutation rules between these operators are

$$[\hat{L}_{AB}, \hat{L}_{AC}] = i g_{AA}\hat{L}_{BC}, \tag{13A.4}$$

where n is the principal quantum number [see (13.198)]. It can be verified that the following combinations of position and momentum operators in a three-dimensional Euclidean space are elements of the Lie algebra of O(4,2):

$$\begin{aligned}
r &= \hat{L}_{56} - \hat{L}_{46},\\
x^i &= \hat{L}_{i5} - \hat{L}_{i4},\\
-i(\mathbf{x}\partial_{\mathbf{x}} + 1) &= \hat{L}_{45},\\
-ir\partial_{x^i} &= \hat{L}_{i6}.
\end{aligned} \tag{13A.5}$$

The last equation follows from the transformation formula [recall (13.138)]

$$\partial_{x^i} = \frac{1}{2\vec{u}^2} e^i{}_\mu \partial_\mu \tag{13A.6}$$

together with

$$\begin{aligned}
u^1 &= \tfrac{1}{2}(z_1 + z_1^*), \quad u^2 = \tfrac{1}{2i}(z_1 - z_1^*),\\
u^3 &= \tfrac{1}{2}(z_2 + z_2^*), \quad u^4 = \tfrac{1}{2i}(z_2 - z_2^*),
\end{aligned} \tag{13A.7}$$

and

$$\partial_1 = (\partial_{z_1} + \partial_{z_1^*}), \quad \partial_2 = i(\partial_{z_1} - \partial_{z_1^*}),$$
$$\partial_3 = (\partial_{z_2} + \partial_{z_2^*}), \quad \partial_4 = i(\partial_{z_2} - \partial_{z_2^*}). \tag{13A.8}$$

Hence

$$-ir\partial_{x^i} = -\frac{i}{2}(\bar{z}\sigma_i\partial_{\bar{z}} + \partial_z\sigma_i z). \tag{13A.9}$$

By analogy with (13A.2), the generators $\hat{L}_{AB}$ can be expressed in terms of the z, z^*-variables as follows:

$$\begin{aligned}
\hat{L}_{ij} &= \tfrac{1}{2}(\bar{z}\sigma_k\partial_{\bar{z}} - \partial_z\sigma_k z),\\
\hat{L}_{i4} &= -\tfrac{1}{2}(\bar{z}\sigma_i z - \partial_z\sigma_i\partial_{\bar{z}}),\\
\hat{L}_{i5} &= \tfrac{1}{2}(\bar{z}\sigma_i z + \partial_z\sigma_i\partial_{\bar{z}}),\\
\hat{L}_{i6} &= -\tfrac{i}{2}(\bar{z}\sigma_i\partial_{\bar{z}} + \partial_z\sigma_i z),\\
\hat{L}_{45} &= -\tfrac{i}{2}(\bar{z}\partial_{\bar{z}} + \partial_z z),\\
\hat{L}_{46} &= -\tfrac{1}{2}(\bar{z}z + \partial_z\partial_{\bar{z}}),\\
\hat{L}_{56} &= \tfrac{1}{2}(\bar{z}z - \partial_z\partial_{\bar{z}}).
\end{aligned} \tag{13A.10}$$

Going over to the operators x^i, ∂_{x^i}, they become

$$\begin{aligned}
\hat{L}_{ij} &= -i(x_i\partial_{x^j} - x_j\partial_{x^i}),\\
\hat{L}_{i4} &= \tfrac{1}{2}\left(-x^i\partial_{\mathbf{x}}^2 - x^i + 2\partial_{x^i}\mathbf{x}\partial_{\mathbf{x}}\right),\\
\hat{L}_{i5} &= \tfrac{1}{2}\left(-x^i\partial_{\mathbf{x}}^2 + x^i + 2\partial_{x^i}\mathbf{x}\partial_{\mathbf{x}}\right),\\
\hat{L}_{i6} &= -ir\partial_{x^i},\\
\hat{L}_{45} &= -i(x^i\partial_{x^i} + 1),\\
\hat{L}_{46} &= \tfrac{1}{2}(-r\partial_{\mathbf{x}}^2 - r),\\
\hat{L}_{56} &= \tfrac{1}{2}(-r\partial_{\mathbf{x}}^2 + r),
\end{aligned} \tag{13A.11}$$

where the purely spatial operators $\partial_{\mathbf{x}}^2$ and $\mathbf{x}\partial_{\mathbf{x}}$ are equal to $\partial_{x^\mu}^2$ and $x^\mu\partial_{x^\mu}$ because of the constraint (13.182).

The Lie algebra of the differential operators (13A.11) is isomorphic to the Lie algebra of the conformal group in four spacetime dimensions, which is an extension of the *inhomogeneous Lorentz group* or *Poincaré group*, defined by the commutators in Minkowski space ($\mu, \nu = 0, 1, 2, 3$), whose metric has the diagonal elements $(+1, -1, -1, -1)$,

$$[P_\mu, P_\nu] = 0, \tag{13A.12}$$
$$[L_{\mu\nu}, P_\lambda] = -i(g_{\mu\lambda}P_\nu - g_{\nu\lambda}P_\mu), \tag{13A.13}$$
$$[L_{\mu\nu}, L_{\lambda\kappa}] = -i(g_{\mu\lambda}L_{\nu\kappa} - g_{\nu\lambda}L_{\mu\kappa} - g_{\mu\kappa}L_{\nu\lambda} - g_{\nu\kappa}L_{\mu\lambda}). \tag{13A.14}$$

The extension involves the generators D of *dilatations* $x^\mu \to \rho x^\mu$ and K_μ of *special conformal transformations*[4]

$$x^\mu \to \frac{x^\mu - c^\mu x^2}{1 - 2cx + c^2x^2}, \tag{13A.15}$$

[4]Note the difference with respect to the conformal transformations à la Weyl in Eq. (13.234). They correspond to local dilatations.

with the additional commutation rules

$$[D, P_\mu] = -iP_\mu, \quad [D, K_\mu] = iK_\mu, \ [D, L_{\mu\nu}] = 0, \tag{13A.16}$$

$$[K_\mu, K_\nu] = 0, \ [K_\mu, P_\nu] = -2i(g_{\mu\nu}D + L_{\mu\nu}), \ [K_\mu, L_{\nu\lambda}] = i(g_{\mu\nu}K_\lambda - g_{\mu\lambda}K_\nu). \tag{13A.17}$$

The commutation rules can be represented by the differential operators

$$\hat{P}_\mu = i\partial_\mu, \quad \hat{M}_{\mu\nu} = i(x_\mu\partial_\nu - x_\nu\partial_\mu), \quad \hat{D} = ix^\mu\partial_\mu, \tag{13A.18}$$

$$\hat{K}_\mu = i(2x_\mu x^\nu\partial_\nu - x^2\partial_\mu). \tag{13A.19}$$

Their combinations

$$J_{\mu\nu} \equiv L_{\mu\nu}, \ J_{\mu 5} \equiv \tfrac{1}{2}(P_\mu - K_\mu), \ J_{\mu 6} \equiv \tfrac{1}{2}(P_\mu + K_\mu), \ J_{56} \equiv D, \tag{13A.20}$$

satisfy the commutation relation of O(4,2):

$$[J_{AB}, J_{CD}] = -i(\bar{g}_{AC}J_{BD} - \bar{g}_{BC}J_{AD} + \bar{g}_{BD}J_{AC} - \bar{g}_{BC}J_{AD}), \tag{13A.21}$$

where the metric $\bar{g}_{AB}$ has the diagonal values $(+1, -1, -1, -1, -1, +1)$.

When working with oscillator wave functions which are factorized in the four u^μ-coordinates, the most convenient form of the generators is

$$\begin{aligned}
\hat{L}_{12} &= i(u^1\partial_2 - u^2\partial_1 - u^3\partial_4 + u^4\partial_3)/2,\\
\hat{L}_{13} &= i(u^1\partial_3 + u^2\partial_4 - u^3\partial_1 - u^4\partial_2)/2,\\
\hat{L}_{14} &= -(u^1u^3 + u^2u^4) + (\partial_1\partial_3 + \partial_2\partial_4)/4,\\
\hat{L}_{15} &= (u^1u^3 + u^2u^4) + (\partial_1\partial_3 + \partial_2\partial_4)/4,\\
\hat{L}_{16} &= -i(u^1\partial_3 + u^2\partial_4 + u^3\partial_1 + u^4\partial_2)/2,\\
\hat{L}_{23} &= i(u^1\partial_4 - u^2\partial_3 + u^3\partial_2 - u^4\partial_1)/2,\\
\hat{L}_{24} &= -(u^1u^4 - u^2u^3) + (\partial_1\partial_4 - \partial_2\partial_3)/4,\\
\hat{L}_{25} &= (u^1u^4 + u^2u^3) + (\partial_1\partial_4 - \partial_2\partial_3)/4,\\
\hat{L}_{26} &= -i(u^1\partial_4 - u^2\partial_3 - u^3\partial_2 + u^4\partial_1)/2,\\
\hat{L}_{34} &= [(u^1)^2 + (u^2)^2 - (u^3)^2 - (u^4)^2]/2 + (\partial_1^2 + \partial_2^2 - \partial_3^2 - \partial_4^2)/8,\\
\hat{L}_{35} &= -[(u^1)^2 + (u^2)^2 - (u^3)^2 - (u^4)^2]/2 + (\partial_1^2 + \partial_2^2 - \partial_3^2 - \partial_4^2)/8,\\
\hat{L}_{36} &= -i(u^1\partial_1 + u^2\partial_2 - u^3\partial_3 - u^4\partial_4)/2,\\
\hat{L}_{45} &= -i(u^1\partial_1 + u^2\partial_2 + u^3\partial_3 + u^4\partial_4 + 2)/2,\\
\hat{L}_{46} &= -(u^\mu)^2/2 - \partial_\mu^2/8,\\
\hat{L}_{56} &= (u^\mu)^2/2 - \partial_\mu^2/8.
\end{aligned} \tag{13A.22}$$

The commutation rules (13A.4) between these generators make the solution of the Schrödinger equation very simple. Rewriting (13.167) as

$$\left(-\frac{a_H}{2}r\boldsymbol{\nabla}^2 - \frac{E}{E_H}\frac{r}{a_H} - 1\right)\psi(\mathbf{x}) = 0, \tag{13A.23}$$

and going to atomic natural units with $a_H = 1, E_H = 1$, we express $r\partial_{\mathbf{x}}^2$ and r in terms of $\hat{L}_{46}, \hat{L}_{56}$ via (13A.11). This gives

$$\left[\frac{1}{2}(\hat{L}_{56} + \hat{L}_{46}) - E(\hat{L}_{56} - \hat{L}_{46}) - 1\right]\psi = 0. \tag{13A.24}$$

With the help of Lie's expansion formula

$$e^{i\hat{A}}\hat{B}e^{-i\hat{A}} = 1 + i[\hat{A}, \hat{B}] + \frac{i^2}{2!}[\hat{A}, [\hat{A}, \hat{B}]] + \ldots$$

for $\hat{A} = \hat{L}_{45}$ and $\hat{B} = \hat{L}_{56}$ and the commutators $[\hat{L}_{45}, \hat{L}_{56}] = iL_{45}$ and $[\hat{L}_{45}, \hat{L}_{46}] = i\hat{L}_{56}$, this can be rewritten as

$$\left[e^{i\vartheta \hat{L}_{45}} \hat{L}_{56} e^{-i\vartheta \hat{L}_{45}} - 1\right] \psi = 0, \tag{13A.25}$$

with

$$\vartheta = \frac{1}{2} \log(-2E). \tag{13A.26}$$

If ψ_n denotes the eigenstates of $\hat{L}_{56}$ with an eigenvalue n, the solutions of (13A.25) are obviously given by the tilted eigenstates $e^{i\vartheta L_{45}} \psi_n$ of the generator $\hat{L}_{56}$ whose eigenvalues are $n = 1, 2, 3, \dots$ [as follows directly from the representation (13A.2)]. For these states, the parameter ϑ takes the values

$$\vartheta = \vartheta_n = -\log n, \tag{13A.27}$$

with the energies $E_n = -1/2n^2$.

Since the energy E in the Schrödinger equation (13A.24) is accompanied by a factor $\hat{L}_{46} - \hat{L}_{56}$, the physical scalar product between Coulomb states is

$$\langle \psi'^H_{n'} | \psi^H_n \rangle_{\rm phys} \equiv \langle \psi'^s_{n'} | (\hat{L}_{56} - \hat{L}_{46}) | \psi^s_n \rangle = \delta_{n'n}. \tag{13A.28}$$

Within this scalar product, the Coulomb wave functions

$$\psi^H_n(\mathbf{x}) = \frac{1}{\sqrt{n}} e^{i\vartheta_n \hat{D}} \psi^s_n(u^\mu) = \frac{1}{\sqrt{n}} \psi^s_n(u^\mu/\sqrt{n}) \tag{13A.29}$$

are orthonormal.

The physical scalar product (13A.28) agrees of course with the scalar product (13.169) and with the scalar product (11.95) derived for a space with torsion in Section 11.4, apart from a trivial constant factor.

It is now easy to calculate the physical matrix elements of the dipole operator x^i and the momentum operator $-i\partial_{x^i}$ using the representations (13A.5). Only operations within the Lie algebra of the group O(4,2) have to be performed. This is why O(4,2) is called the *dynamical group* of the Coulomb system [13].

For completeness, let us state the relation between the states in the oscillator basis $|n_1 n_2 m\rangle$ and the eigenstates of a fixed angular momentum $|nlm\rangle$ of (13.219), which is analogous to the combination (13.254)

$$\begin{aligned} |nlm\rangle &= \sum_{n_1+n_2+m=(n-1)/2} \\ &\times |n_1 n_2 m\rangle \langle \tfrac{1}{2}(n-1), \tfrac{1}{2}(n_2 - n_1 + m); \tfrac{1}{2}(n-1), \tfrac{1}{2}(n_1 - n_2 + m) | l, m\rangle. \end{aligned} \tag{13A.30}$$

Appendix 13B Wave Functions in Three-Dimensional Momentum Space

Let us introduce the Bohr momentum $p_H \equiv \hbar/a_H = Me^2/\hbar$ and go to units where $p_H = 1$. Then the radial wave functions $F_{nl}(p)$ with unit normalization $\int_0^\infty dp\, p^2 F^2_{nlm}(p) = 1$ are given by []

$$F_{nl}(p) = \sqrt{\frac{2}{\pi}} \sqrt{\frac{(n-l-1)!}{(n-l)!}} n^2 2^{2(l+1)} l! \frac{n^l p^l}{(n^2p^2+1)^{l+2}} C^{(l+1)}_{n-l-1}\left(\frac{n^2p^2-1}{n^2p^2+1}\right), \tag{13B.31}$$

where $C^{(\lambda)}_n(z)$ are the Gegenbauer polynomials defined in (8.102), for example

$$C^{(\lambda)}_0(z) = 1, \quad C^{(\lambda)}_1(z) = 2\lambda z, \quad C^{(\lambda)}_2(z) = 2\lambda(\lambda+1)z^2 - \lambda, \dots . \tag{13B.32}$$

The lowest wave functions are

$$F_{10} = 4\sqrt{\frac{2}{\pi}}\frac{1}{(p^2+1)^2}, \quad F_{20} = \frac{32}{\sqrt{\pi}}\frac{4p^2-1}{(4p^2+1)^3}, \quad F_{21} = \frac{128}{\sqrt{3\pi}}\frac{p}{(4p^2+1)^3}. \tag{13B.33}$$

In two dimensions, the momentum space wave functions were listed in Ref. [21].

Notes and References

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