Canonical Transformations and the Radial Oscillator and Coulomb Problems*

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In a previous paper a discussion was given of linear canonical transformations and their unitary representation. We wish to extend this analysis to nonlinear canonical transformations, particularly those that are relevant to physically interesting many-body problems. As a first step in this direction we discuss the nonlinear canonical transformations associated with the radial oscillator and Coulomb problems in which the corresponding Hamiltonian has a centrifugal force of arbitrary strength. By embedding the radial oscillator problem in a higher dimensional configuration space, we obtain its dynamical group of canonical transformations as well as its unitary representation, from the $Sp(2)$ group of linear transformations and its representation in the higher-dimensional space. The results of the Coulomb problem can be derived from those of the oscillator with the help of the well-known canonical transformation that maps the first problem on the second in two-dimensional configuration space. Finally, we make use of these nonlinear canonical transformations, to derive the matrix elements of powers of r in the oscillator and Coulomb problems from a group theoretical standpoint.

1. INTRODUCTION

In previous publications,[1-3] we discussed the role of canonical transformations in quantum mechanics, and when the transformations were linear we obtained their unitary representations in appropriate spaces. These representations have also been derived by other authors from a more abstract standpoint.[4]

As our eventual aim is to obtain relevant canonical transformations and their unitary representations for physically significant many-body problems,[3] we must first deal with problems of one particle in one dimension that go beyond the harmonic oscillator case,[1] which was the starting point of our discussion. Thus in this paper we derive explicitly the dynamical Lie group (and not only the Lie algebra as is customary in the literature) of canonical transformations of the radial oscillator and Coulomb problems in which we have a centrifugal force of arbitrary strength. We then proceed to obtain the unitary representation of this group in configuration space and in the basis in which the Hamiltonian H is diagonal, and finally determine, as a group theoretical problem, the matrix elements of powers of the radial coordinate with respect to eigenstates of H.

By embedding our one-dimensional radial oscillator in a two-dimensional configuration space, we easily derive its dynamical group and the corresponding unitary representation from particular linear canonical transformations in the four-dimensional phase space of the latter problem. The well-known mappings[3,5] between the two-dimensional oscillator and Coulomb problems, allows us then to translate our results to the radial Coulomb case in a straightforward fashion.

2. THE RADIAL OSCILLATOR PROBLEM

We wish to consider a single particle one-dimensional problem whose Hamiltonian (in units in which the mass, frequency of the oscillator and $\hbar$ are 1) is

$$H = \tfrac{1}{2}(p_r^2 + \lambda^2 r^{-2} + r^2) \tag{2.1}$$

The coordinate r varies in the interval $0 \le r < \infty$, p_r is its canonically conjugate momentum, and λ is an arbitrary real constant. For reasons that will appear later we shall denote by μ a real positive constant related to λ through

$$\mu = (\lambda^2 + \tfrac{1}{4})^{1/2} \quad \text{or} \quad \lambda^2 = (\mu - \tfrac{1}{2})[(\mu - \tfrac{1}{2}) + 1]. \tag{2.2}$$

As the Poisson bracket $\{r, p_r\}$ is 1, we conclude that in the quantum mechanical picture $p_r = -i\partial/\partial r$ and thus the eigenstates $f(r)$ of (2.1) satisfy the equation

$$\frac{1}{2}\left(-\frac{d^2}{dr^2} + \frac{\lambda^2}{r^2} + r^2\right)f(r) = Ef(r). \tag{2.3}$$

It is well known that the eigenstates of (2.3) characterized by μ and an integer n have the form

$$f_n^\mu(r) \equiv [2(n!)]^{1/2}[\Gamma(n + \mu + 1)]^{-1/2} e^{-r^2/2} r^{\mu+1/2} L_n^\mu(r^2), \tag{2.4a}$$

where[6] L_n^μ is an associated Laguerre polynomial, and λ and μ are related as in (2.2). The states (2.4a) are orthonormal in the sense

$$\int_0^\infty f_{n'}^\mu(r) f_{n''}^\mu(r) dr = \delta_{n'n''}, \tag{2.4b}$$

and the eigenvalues of (2.3) are given by

$$E_n = (2n + \mu + 1), \quad n \text{ nonnegative integer.} \tag{2.5}$$

A. The Dynamical Group of Canonical Transformations

We wish now to obtain explicitly the dynamical Lie group associated with the Hamiltonian (2.1), and its unitary representation both in configuration space and in the basis where H is diagonal. For this purpose let us first replace λ in (2.1) by a momentum p_θ associated with an angle θ; we have then the two-dimensional Hamiltonian for an oscillator problem which in polar and cartesian coordinates takes the form

$$\mathbf{H} \equiv \tfrac{1}{2}(p_r^2 + r^{-2}p_\theta^2 + r^2) = \tfrac{1}{2}(\mathbf{p}^2 + \mathbf{r}^2) = \tfrac{1}{2}(p_1^2 + x_1^2 + p_2^2 + x_2^2). \tag{2.6}$$

We first recall[1,2] that the dynamical group of canonical transformations of $\mathbf{H}$ is the symplectic group in four dimensions $Sp(4)$. This group has a subgroup

$$Sp(4) \supset Sp(2) \times O(2), \tag{2.7}$$

where $O(2)$ is the rotation group in the two-dimensional space, while $Sp(2)$ is the symplectic group of linear canonical transformations

$$\bar{\mathbf{r}} = a\mathbf{r} + b\mathbf{p}, \quad \bar{\mathbf{p}} = c\mathbf{r} + d\mathbf{p}, \quad ad - bc = 1, \tag{2.8}$$

in which the constants a, b, c, d are real.

We now note that under the transformation (2.8) the angular momentum

$$p_\theta \equiv x_1 p_2 - x_2 p_1 \tag{2.9}$$

remains invariant. As, furthermore, we have that

$$\mathbf{r}\cdot\mathbf{p} = rp_r, \quad \mathbf{p}^2 = p_r^2 + r^{-2}p_\theta^2. \tag{2.10}$$

We see that the transformation (2.8) implies that the new radial coordinate and momentum $\bar{r}, \bar{p}_r$ are given in terms of the old ones r, p_r by

$$\bar{r} = [a^2r^2 + b^2(p_r^2 + \lambda^2 r^{-2}) + 2abrp_r]^{1/2}, \qquad (2.11a)$$

$$\bar{p}_r = \frac{acr^2 + bd(p_r^2 + \lambda^2 r^{-2}) + (ad + bc)rp_r}{[a^2r^2 + b^2(p_r^2 + \lambda^2 r^{-2}) + 2abrp_r]^{1/2}}, \qquad (2.11b)$$

where we replaced $p_\theta = \bar{p}_\theta$ by a constant value λ.

We have thus obtained the dynamical Lie group associated with the Hamiltonian (2.1) which is a representation of the group of unimodular real matrices

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad ad - bc = 1. \qquad (2.12)$$

The subgroup $O(2)$ of (2.12) (not to be confused with the rotation group in two dimensions) for which

$$a = d = \cos\tfrac{1}{2}\alpha, \quad b = -c = \sin\tfrac{1}{2}\alpha, \qquad (2.13)$$

is the symmetry group of the Hamiltonian (2.1) as can be checked directly. We wish to determine the unitary representation of the canonical transformations (2.11) in a basis in which r is diagonal.

B. The Unitary Representation of the Dynamical Group in Configuration Space

We shall limit our discussion to the transformations (2.11) in which $b > 0$. The case $b < 0$ follows immediately[1,2] from it as well as the limit $b \to 0$. The analysis in Ref. 2 then indicates that for the group of linear canonical transformations (2.8) of the two-dimensional oscillator (2.6), the unitary representation is

$$\begin{aligned}\langle \mathbf{r}' | U | \mathbf{r}'' \rangle &= (2\pi b)^{-1} \exp[(-i/2b) \\ &\quad \times (ar'^2 - 2\mathbf{r}'\cdot\mathbf{r}'' + dr''^2)] \\ &= (2\pi b)^{-1} \exp[(-i/2b)(ar'^2 + dr''^2)] \\ &\quad \times \sum_{m=-\infty}^{\infty} i^m J_m(b^{-1}r'r'') e^{im(\theta'-\theta'')}, \end{aligned} \qquad (2.14)$$

where in the last term we have expanded the two-dimensional plane wave in polar coordinates.[7]

The eigenstates of the two-dimensional oscillator (2.6) in polar coordinates are characterized by the integer quantum numbers n, m and have the explicit form

$$\langle \mathbf{r} | nm \rangle = r^{-1/2} f_n^{|m|}(r) (2\pi)^{-1/2} e^{im\theta}, \qquad (2.15)$$

where the radial function is given by (2.4a) with $\mu = (\lambda^2 + \frac{1}{4})^{1/2}$ being replaced by $|m|$. The unitary representation (2.14) with respect to these states is clearly diagonal in the m index as (2.14) is invariant under rotations and, thus, we can write

$$\begin{aligned}\langle n'm | U | n''m \rangle &= \iint \langle n'm | \mathbf{r}' \rangle d\mathbf{r}' \langle \mathbf{r}' | U | \mathbf{r}'' \rangle d\mathbf{r}'' \langle \mathbf{r}'' | n''m \rangle \\ &= \int_0^\infty \int_0^\infty f_{n'}^{|m|}(r') dr' \{ i^m b^{-1} \\ &\quad \times (r'r'')^{1/2} J_m(b^{-1}r'r'') \exp[(-i/2b) \\ &\quad \times (ar'^2 + dr''^2)] \} dr'' f_{n''}^{|m|}(r''). \end{aligned} \qquad (2.16)$$

This equation immediately suggests that for $\mu = |m|$ or $\lambda = (m^2 - \frac{1}{4})^{1/2}$ the unitary representation between the radial variables $\langle r' | U_\mu | r'' \rangle$ of the canonical transformation (2.11) [which explicitly depends on μ through (2.2)] is given by the expression inside the curly bracket of (2.16). Thus we may expect that for an arbitrary μ we have for the unitary representation of (2.11)

$$\langle r' | U_\mu | r'' \rangle = b^{-1}(r'r'')^{1/2} J_\mu(b^{-1}r'r'') \times \exp[(-i/2b)(ar'^2 + dr''^2)]. \qquad (2.17)$$

We suppressed the i^μ in (2.17) as, in any case, our representations will be ray representations.[1,2,8]

While (2.17) is rigorously true for $\mu = |m|$, it is only a surmise for other values of μ. We proceed to justify it by obtaining explicitly the unitary representation for arbitrary μ in the basis in which the Hamiltonian (2.1) is diagonal.

C. Unitary Representations of Canonical Transformations in the Basis in Which H Is Diagonal

If we want to have the unitary representation (2.17) in a basis in which H is diagonal, we must calculate the integral

$$\langle n' | U_\mu | n'' \rangle = \int_0^\infty \int_0^\infty f_{n'}^\mu(r') dr' \langle r' | U_\mu | r'' \rangle dr'' f_{n''}^\mu(r'') \qquad (2.18)$$

This integral can be evaluated by exactly the same procedure that was followed in the determination of the matrix element (4.34) in Ref. 2. In fact, we just need to replace l by $\mu - \frac{1}{2}$ and suppress the factor i^l to get the value of the double integral (2.18).

To justify now the value (2.17) for $\langle r' | U_\mu | r'' \rangle$ for arbitrary μ, we notice first that the most general matrix (2.12) of the symplectic group can be written as[1]

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} \cos\frac{1}{2}\alpha & \sin\frac{1}{2}\alpha \\ -\sin\frac{1}{2}\alpha & \cos\frac{1}{2}\alpha \end{pmatrix} \begin{pmatrix} e^{1/2\beta} & 0 \\ 0 & e^{-1/2\beta} \end{pmatrix} \times \begin{pmatrix} \cos\frac{1}{2}\gamma & \sin\frac{1}{2}\gamma \\ -\sin\frac{1}{2}\gamma & \cos\frac{1}{2}\gamma \end{pmatrix}. \qquad (2.19)$$

The transformations associated with the angles α and γ leave the Hamiltonian (2.1) invariant and thus from a classical standpoint we could identify these angles with time. Therefore when the elements of the matrix (2.19) are given by

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{pmatrix}, \qquad (2.20)$$

the transformation (2.11) gives us the coordinate and momentum at time t from the coordinate and momentum at time 0. The corresponding unitary representation in the basis in which the Hamiltonian is diagonal must then be

$$\langle n' | U_\mu | n'' \rangle_{\alpha=2t,\beta=\gamma=0} = \delta_{n'n''} \exp[i(2n' + \mu + 1)t], \qquad (2.21)$$

as the energy is given by (2.5). From (4.37) in Ref. 2 we note that we get exactly this value when we replace l by $\mu - (1/2)$ except for a constant phase which is irrelevant because we deal with ray representations. Thus the integral (2.18) gives the correct unitary representation for any canonical transformation (2.11) in which the symplectic matrix has the form (2.20).

It remains then to check only if the integral (2.18) gives the unitary representation for a dilatation in which

$$a = d^{-1} = e^{\beta/2}, \quad b = c = 0. \tag{2.22}$$

Using the formula[6]

$$L_n^\mu(e^\beta x^2) = \sum_{k=0}^{n} [k!\,\Gamma(n-k+\mu+1)]^{-1}\Gamma(n+\mu+1) \times e^{(n-k)\beta}(1-e^\beta)^k L_{n-k}^\mu(x^2), \tag{2.23}$$

we can immediately find out the expansion of the states

$$e^{-\beta/4} f_n^\mu(e^{\beta/2} r), \tag{2.24}$$

in terms of the states $f_n^\mu(r)$ of (2.4). The result turns out to be

$$\begin{aligned}\langle n'|U_\mu|n''\rangle_{\alpha=0,\beta,\gamma=0} &= i^{-\mu-1}[n'!\,n''!\,\Gamma(n'+\mu+1) \\ &\times \Gamma(n''+\mu+1)]^{1/2}(\cosh\tfrac{1}{2}\beta)^{-\mu-1} \\ &\times (1-e^\beta)^{n'+n''}(1+e^\beta)^{-n'-n''} \\ &\times \sum_p \{[p!\,(n'-p)!\,(n''-p)!\,\Gamma(p+\mu+1)]^{-1} \\ &\times (-1)^{n'-p}(\sinh\tfrac{1}{2}\beta)^{-2p}\},\end{aligned} \tag{2.25}$$

and up to a phase it is identical[2] to the one that comes out from the integral (2.18).

We have thus proved that (2.17) is the unitary representation in configuration space of the group of canonical transformations (2.11) for arbitrary $\lambda = (\mu^2 - \frac{1}{4})^{1/2}$. The unitary representation in a basis in which the Hamiltonian is diagonal is given by products of the matrices (2.21) and (2.25) using the decomposition (2.19).

3. THE RADIAL COULOMB PROBLEM

We now wish to consider a Hamiltonian which in atomic units has the form

$$\mathcal{H} = \tfrac{1}{2}(p_r^2 + \Lambda^2 r^{-2}) - r^{-1}, \tag{3.1}$$

with r, p_r having the same meaning as in Sec. 2 and Λ being an arbitrary real constant. As in (2.2) we introduce a positive constant M related to Λ through

$$\mathrm{M} \equiv (\Lambda^2 + \tfrac{1}{4})^{1/2} \quad \text{or} \quad \Lambda^2 = (M - \tfrac{1}{2})[(M - \tfrac{1}{2}) + 1]. \tag{3.2}$$

We shall denote the eigenvalue of the Hamiltonian (3.1) by

$$E \equiv -(2\nu^2)^{-1}. \tag{3.3a}$$

Introducing then the variable

$$\rho = (r/\nu), \tag{3.3b}$$

we see that the eigenstates of (3.1) satisfy the equation

$$\rho\left[\left(-\frac{d^2}{d\rho^2} + \frac{\Lambda^2}{\rho^2}\right) + 1\right]F(\rho) = 2\nu F(\rho). \tag{3.4}$$

The analysis of this equation indicates that the solutions will be regular at ∞ only when

$$\nu = n + \mathrm{M} + \tfrac{1}{2}, \tag{3.5}$$

with the radial quantum number n being a nonnegative integer. The eigenstates have then the explicit form

$$F_n^{\mathrm{M}}(\rho) = A_{n\mathrm{M}}\,\rho^{\mathrm{M}+1/2} e^{-\rho} L_n^{2\mathrm{M}}(2\rho), \tag{3.6}$$

where[6] $L_n^{2\mathrm{M}}$ are associated Laguerre polynomials in which M and n are related to Λ and ν through (3.2) and (3.5).

The coefficient $A_{n\mathrm{M}}$ can be determined by normalizations which can be achieved in two ways. If we consider F_n^{M} as a function of r, the requirement

$$\int_0^\infty F_{n'}^{\mathrm{M}}(r/\nu') F_{n''}^{\mathrm{M}}(r/\nu'')\,dr = \delta_{n'n''} \tag{3.7a}$$

gives

$$A_{n\mathrm{M}} \equiv A_{n\mathrm{M}}^c = \left[\frac{2^{2\mathrm{M}+1}(n-1)!}{(n+\mathrm{M}+\frac{1}{2})\Gamma(2\mathrm{M}+n+1)}\right]^{1/2}. \tag{3.7b}$$

On the other hand, if we consider F_n^{M} as a function of ρ, the operator on the left-hand side of (3.4) will be Hermitian (and thus give rise to orthonormalization), only for integrals of the form

$$\int_0^\infty F_{n'}^{\mathrm{M}}(\rho) F_{n''}^{\mathrm{M}}(\rho)\rho^{-1}\,d\rho = \delta_{n'n''}, \tag{3.8a}$$

which implies that the normalization coefficient becomes

$$A_{n\mathrm{M}} \equiv A_{n\mathrm{M}}^p = 2^{\mathrm{M}}[2(n!)/\Gamma(n+2M+1)]^{1/2}. \tag{3.8b}$$

The upper indices c and p distinguish between the two cases when necessary. When referring to the function $F_n^{\mathrm{M}}(\rho)$ without qualifications, we shall understand that it is given by (3.6) with the normalization (3.8b).

We wish now to obtain explicitly the dynamical Lie group associated with the problem (3.4) as well as its unitary representation. We can achieve both objectives through the mappings between the two-dimensional oscillator and Coulomb problems.

A. Mappings between the Two-Dimensional Oscillator and Coulomb Problems

From the two-dimensional coordinate and momentum vectors $\mathbf{r}, \mathbf{p}$ we can build the following independent quadratic expressions[1,2]

$$\begin{aligned} I_1 &\equiv \tfrac{1}{4}(\mathbf{p}^2 - \mathbf{r}^2), \quad I_2 \equiv \tfrac{1}{4}(\mathbf{r}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{r}), \\ I_3 &\equiv \tfrac{1}{4}(\mathbf{p}^2 + \mathbf{r}^2) = \tfrac{1}{2}H. \end{aligned} \tag{3.9}$$

The Poisson brackets between the I_i, either when they are considered as classical observables or quantum mechanical operators, are given by

$$\{I_1, I_2\} = -I_3, \quad \{I_3, I_1\} = I_2, \quad \{I_2, I_3\} = I_1. \tag{3.10}$$

Thus they correspond to the generators[9] of a Lie algebra of the group $SU(1,1)$, which is isomorphic[1,3] to the $Sp(2)$ group of linear canonical transformations (2.8).

Turning now our attention to the two-dimensional Coulomb problem, we describe it in terms of the radial coordinate ρ and an angle φ. The corresponding Cartesian coordinates we designate by

$$\xi_1 = \rho \cos\varphi, \quad \xi_2 = \rho \sin\varphi \tag{3.11}$$

and their canonically conjugate momenta by π_1, π_2.

In terms of the two-dimensional vectors $\boldsymbol{\xi}, \boldsymbol{\pi}$ we can now construct the expressions[10]

$$K_1 \equiv \tfrac{1}{2}\rho(\boldsymbol{\pi}^2 - 1), \quad K_2 \equiv \tfrac{3}{4}\boldsymbol{\xi}\cdot\boldsymbol{\pi} + \tfrac{1}{4}\boldsymbol{\pi}\cdot\boldsymbol{\xi},$$
$$K_3 \equiv \tfrac{1}{2}\rho(\boldsymbol{\pi}^2 + 1). \tag{3.12}$$

The Poisson brackets between the K_i, both classically and quantum mechanically, are given by

$$\{K_1, K_2\} = -K_3, \quad \{K_3, K_1\} = K_2, \quad \{K_2, K_3\} = K_1. \tag{3.13}$$

Thus they correspond to the generators[9] of the Lie algebra of $SU(1,1)$. The operators K_i are Hermitian under the measure used in (3.8a).

Before proceeding with the explicit construction of the group whose generators are the K_i of (3.13), we first indicate why we are interested in it. When we write K_3 as a quantum mechanical operator in polar coordinates, we immediately notice that its eigenstates are given by the wavefunction

$$\psi(\rho, \varphi) = \rho^{-1/2}F(\rho)e^{i\mathrm{M}\varphi}, \tag{3.14}$$

in which $F(\rho)$ satisfies Eq. (3.4) with $\mathrm{M} = (\Lambda^2 + \frac{1}{4})^{1/2}$ being an integer. Thus the relation of the problem (3.4) with the Lie algebra (3.13) is exactly of the same type as the one that exists between the radial equation (2.3) for the harmonic oscillator and the Lie algebra whose generators are the I_i given by (3.9). As the latter relation allowed us to determine,[1–3] the group of canonical transformations and its unitary representation for the harmonic oscillator problem, we expect that the former relation will achieve the same objectives for the Coulomb problem.

We now consider a canonical transformation that converts the I_i of (3.9) into K_i of (3.12) assuming them to be classical observables. The mapping appears in its simplest form in polar coordinates if we consider the relations[3,5]

$$r^2 = 2\rho, \tag{3.15a}$$

$$\theta = \tfrac{1}{2}\varphi \tag{3.15b}$$

This implies that in Cartesian coordinates we have

$$\xi_1 = \tfrac{1}{2}(x_1^2 - x_2^2), \tag{3.16a}$$

$$\xi_2 = x_1 x_2. \tag{3.16b}$$

To determine the corresponding relation for momenta we recall that in classical mechanics the generalized velocities and momenta are connected by Hamilton's equation

$$\dot{q}_i = \partial H/\partial p_i. \tag{3.17}$$

For the two-dimensional oscillator and Coulomb problems the H are, respectively, $2I_3$ and $2K_3$ and thus

$$p_i = \dot{x}_i, \quad \pi_i = \dot{\xi}_i/2\rho, \quad i = 1, 2. \tag{3.18}$$

From (3.16a) and (3.16b) we obtain then that

$$\pi_1 = r^{-2}(x_1 p_1 - x_2 p_2), \tag{3.16c}$$

$$\pi_2 = r^{-2}(x_1 p_2 + x_2 p_1). \tag{3.16d}$$

We easily check that the transformation (3.16) is canonical and besides it maps the generators I_i of (3.9) of the Lie Algebra of the harmonic oscillator into the K_i of (3.12) of the Coulomb problem. From (3.16) we note also that

$$\pi_\varphi = \xi_1\pi_2 - \xi_2\pi_1 = \tfrac{1}{2}(x_1p_2 - x_2p_1) = \tfrac{1}{2}p_\theta, \tag{3.19a}$$

$$\rho\pi_\rho = \boldsymbol{\xi}\cdot\boldsymbol{\pi} = \tfrac{1}{2}\mathbf{r}\cdot\mathbf{p} = \tfrac{1}{2}rp_r, \tag{3.19b}$$

$$\boldsymbol{\pi}^2 = \mathbf{p}^2/r^2. \tag{3.19c}$$

In particular the transformation (3.15) maps I_i on K_i even when we interpret them as quantum mechanical operators.

With the help of the canonical transformations (3.15) and (3.19), we are now in position to obtain the dynamical group of canonical transformations associated with problem (3.4).

B. The Dynamical Group of the Coulomb Problem and Its Unitary Representation

The dynamical group of canonical transformations associated with the harmonic oscillator problem is given by (2.11). In the Coulomb problem our radial variable is ρ and its corresponding momentum π_ρ. From the relations (3.15) and (3.19) connecting ρ, π_ρ and r, p_r we conclude that (2.11) gives rise to the following nonlinear canonical transformations for the Coulomb problem

$$\bar{\rho} = \tfrac{1}{2}\bar{r}^2 = \tfrac{1}{2}(a^2r^2 + b^2p^2 + 2ab\mathbf{r}\cdot\mathbf{p})$$
$$= \rho[(a + b\pi_\rho)^2 + b^2\Lambda^2\rho^{-2}], \tag{3.20a}$$

$$\bar{\pi}_\rho = \bar{\rho}^{-1}\bar{\boldsymbol{\xi}}\cdot\bar{\boldsymbol{\pi}} = \frac{(a + b\pi_\rho)(c + d\pi_\rho) + bd\Lambda^2\rho^{-2}}{(a + b\pi_\rho)^2 + b^2\Lambda^2\rho^{-2}}, \tag{3.20b}$$

where we have replaced $\pi_\varphi = \bar{\pi}_\varphi$ by the value Λ; it takes in the classical picture. Thus we have obtained the dynamical Lie group of canonical transformations associated with the Coulomb system in the formulation (3.4).

To discuss the unitary representation of the canonical transformation (3.20), we first notice that from (3.15a) and (3.19b) we can map the classical oscillator problem (2.1) with $\lambda = 2\Lambda$, onto the Hamiltonian

$$\rho(\pi_\rho^2 + \Lambda^2\rho^{-2} + 1), \tag{3.21}$$

with the help of the canonical transformations

$$\rho = \tfrac{1}{2}r^2, \tag{3.22a}$$

$$\pi_\rho = r^{-1}p_r. \tag{3.22b}$$

Thus if we obtain the unitary representation V associated with (3.22), we can determine the corresponding one for (3.20) through the similarity transformation

$$W_{\mathrm{M}} \equiv V^{-1}U_\mu V, \tag{3.23}$$

where the matrix elements of U_μ are given by (2.17). In this expression we have to use the relation $\mu = 2\mathrm{M}$, which is the quantum mechanical equivalent of $\lambda = 2\Lambda$, as in quantum mechanics μ and M are, respectively, the eigenvalues of p_θ and π_φ related by $p_\theta = 2\pi_\varphi$ as indicated in the previous subsection.

To get V, we proceed as in Refs. 1 and 2. Using the Dirac notation in which we indicate by $\langle r'|, |r''\rangle$ and $(\rho'|, |\rho'')$ bras and kets in which r and ρ are, respectively, diagonal, we look for the transformation bracket $\langle r'|\rho')$ that satisfies the equation[1,2]

$$\rho\langle r'|\rho') = \rho'\langle r'|\rho'). \tag{3.24}$$

From (3.22a) this equation implies that the transformation bracket is proportional to $\delta(\rho' - \frac{1}{2}r'^2)$. If we further require that the bracket should be orthonormal in the sense

$$\int_0^\infty (\rho'|r'\rangle dr'\langle r'|\rho'') = \delta(\rho' - \rho''), \tag{3.25}$$

we obtain that

$$\langle r'|\rho') = (2\rho')^{1/4}\delta(\rho' - \tfrac{1}{2}r'^2). \tag{3.26}$$

We can multiply the expression (3.26) by any phase factor which is a function of ρ'; but this proves unnecessary as the transformation bracket (3.26) already guarantees that

$$(\rho'|\rho|\rho'') = \int (\rho'|r'\rangle \tfrac{1}{2}r'^2\langle r'|\rho'')dr' = \rho'\delta(\rho' - \rho''), \tag{3.27a}$$

$$\begin{aligned}(\rho'|\pi_\rho|\rho'') &= \int (\rho'|r'\rangle\left[\left(\frac{1}{ir'}\frac{\partial}{\partial r'} + \frac{i}{2r'^2}\right)\langle r'|\rho'')\right]dr' \\ &= \int (\rho'|r'\rangle\left(-\frac{1}{i}\frac{\partial}{\partial\rho''}\langle r'|\rho'')\right)dr' \\ &= -\frac{1}{i}\frac{\partial}{\partial\rho''}\,\delta(\rho' - \rho''),\end{aligned} \tag{3.27b}$$

where we made use of the fact that the Hermitian form of the quantum mechanical operator π_ρ of (3.22b) is

$$\tfrac{1}{2}(r^{-1}p_r + p_r r^{-1}) = \frac{1}{ir}\frac{\partial}{\partial r} + \frac{i}{2r^2}. \tag{3.27c}$$

The unitary representation of the canonical transformation (3.22) is thus given by the bracket (3.26) and therefore the matrix element of $V^{-1}U_{2M}V$ in the representation in which ρ is diagonal takes the form

$$\begin{aligned}(\rho'|W_M|\rho'') &= (\rho'|V^{-1}U_{2M}V|\rho'') \\ &= \iint (\rho'|r'\rangle dr'\langle r'|U_{2M}|r''\rangle dr''\langle r''|\rho'').\end{aligned} \tag{3.28}$$

Substituting the values (2.17) for $\langle r'|U_{2M}|r''\rangle$ and (3.26) for $\langle r'|\rho')$, we obtain

$$\begin{aligned}(\rho'|W_M|\rho'') = b^{-1}J_{2M}[2b^{-1}(\rho'\rho'')^{1/2}] \\ \times \exp[(-i/b)(a\rho' + d\rho'')].\end{aligned} \tag{3.29}$$

The unitary representation when the Hamiltonian (3.21) is diagonal, rather than the observable ρ, is given by

$$\begin{aligned}(n'|W_M|n'') = \int_0^\infty\int_0^\infty \rho'^{-1/2}F^M_{n'}(\rho') \\ \times d\rho'(\rho'|W_M|\rho'')d\rho''\rho''^{-1/2}F^M_{n''}(\rho''),\end{aligned} \tag{3.30}$$

where $F^M_n(\rho)$ is given by (3.6) and the extra factors $\rho'^{-1/2}, \rho''^{-1/2}$ come from the normalization (3.8). As from (2.4a) and (3.6) we have that

$$F^M_n(\rho) = (\rho/2)^{1/4}f^{2M}_n[(2\rho)^{1/2}], \tag{3.31}$$

we immediately obtain that

$$(n'|W_M|n'') = \langle n'|U_{2M}|n''\rangle, \tag{3.32}$$

with the latter expression being given by (2.21) when the transformation is of the type (2.20) and has the form (2.25) for a dilatation.

It is important to keep in mind that our canonical transformations and their representations are not so much connected with the Coulomb problem (3.1) as with the one whose Hamiltonian is (3.21). The latter is directly related, when $\Lambda^2 = l(l+1)$, with the stereographic projection of a four-dimensional point rotor on a three-dimensional momentum space as was first pointed out by Fock.[11] Thus we shall refer to the problem whose Hamiltonian is (3.21) as the pseudo-Coulomb problem and our analysis, so far, has been restricted to it.

4. RADIAL MATRIX ELEMENTS

The matrix elements of powers of the radial coordinate with respect to oscillator or Coulomb wavefunctions are easily evaluated using properties of the Laguerre polynomials or their generating functions.[6] We wish though to obtain their values through the use of the dynamical group of canonical transformations so as to develop a procedure susceptible to generalization to more complex problems.

For the oscillator case the radial integrals were already determined through the use of the dynamical group of canonical transformations[12] as well as by other group theoretical approaches.[13] We have thus to concentrate on the Coulomb problem, on which group theoretical methods have been developed,[14] but they do not use canonical transformations. Rather than enter into this problem directly it will prove more effective to discuss first the matrix elements of r^{2k}, k integer, in the oscillator problem, from an angle different from the one used in Ref. 12. Once we determine these matrix elements the extension to the pseudo-Coulomb problem will be achieved through the mappings (3.22a) and (3.31), while the actual Coulomb integrals of r^k can be obtained from those of the pseudo-Coulomb problem and the expression (2.25) for dilatations.

A. Matrix Elements of r^{2k} for Oscillator States

We start our discussion by noticing that if in the generators (3.9) of the dynamical group of the two-dimensional oscillator, we replace

$$p^2 = p_r^2 + r^{-2}p_\theta^2, \quad p_\theta = \lambda, \tag{4.1}$$

we get the observables

$$\begin{aligned}I_1 &= \tfrac{1}{4}(p_r^2 + \lambda^2 r^{-2} - r^2), \quad I_2 = \tfrac{1}{4}(rp_r + p_r r), \\ I_3 &= \tfrac{1}{4}(p_r^2 + \lambda^2 r^{-2} + r^2).\end{aligned} \tag{4.2}$$

The Poisson brackets of the I_i, both classically and quantum mechanically, have the value (3.10) and thus these observables are the generators of Lie Algebra of a group $Sp(2)$ as well as groups isomorphic to it[1] such as $SU(1,1)$.

From I_1 and I_2 we can construct the operators

$$I_\pm \equiv I_i \pm iI_2 \tag{4.3}$$

and we easily check that for the $f_n^\mu(r)$ of (2.4a) we have

$$I_\pm f_n^\mu(r) = [(n+\mu+\tfrac{1}{2}\pm\tfrac{1}{2})(n+\tfrac{1}{2}\pm\tfrac{1}{2})]^{1/2} f_{n\pm1}^\mu(r). \tag{4.4}$$

Thus $I_\pm$ are raising and lowering operators for the index n and the set of $f_n^\mu(r), n = 0, 1, 2, \ldots$, belong to a single unitary irreducible representation of the $SU(1,1)$ group. The lowest weight element of the set corresponds to $n = 0$ and, thus, is an eigenstate of I_3 with eigenvalues $\frac{1}{2}(\mu+1)$. We can use this number or more compactly μ itself to label the irreducible representation. If μ is 0 or a positive integer, the representations are part of the discrete series discussed by Bargmann[9]: They are single valued on the $SU(1,1)$ group manifold and are characterized by the integer or semi-integer numbers

$$\tfrac{1}{2}(\mu+1) = \tfrac{1}{2}, 1, \tfrac{3}{2}, 2, \tfrac{5}{2}, \cdots. \tag{4.5}$$

When μ is an arbitrary nonnegative real number the representations are multiple valued on the $SU(1,1)$ group manifold and are not discussed in Bargmann's paper; but they are as straightforward to obtain as those when μ is integer. In fact, a basis for multi-valued-irreducible representations for arbitrary μ is precisely given by the functions $f_n^\mu(r), n = 0, 1, 2, \ldots$, with μ specifying the irreducible representation and n indicating its row.

We wish now to characterize r^{2k} as a linear combination of irreducible tensors of $SU(1,1)$. When we achieve this purpose we can make use of the Wigner–Eckart theorem to express the matrix elements of r^{2k} in terms of the Wigner coefficients of $SU(1,1)$ determined by Ui.[15] To reach our objective we notice from (4.2) that

$$\tfrac{1}{2}r^2 = I_3 - I_1. \tag{4.6}$$

Thus r^{2k} can be expressed as a polynomial in the generators I_i of the dynamical group. To develop this polynomial in terms of irreducible tensors of $SU(1,1)$, we first introduce the auxiliary generators

$$I_1' \equiv iI_1, \quad I_2' \equiv iI_2, \quad I_3' \equiv I_3. \tag{4.7}$$

The $SU(1,1)$ Casimir operator can then be written as

$$I_3^2 - I_1^2 - I_2^2 = I_1'^2 + I_2'^2 + I_3'^2, \tag{4.8}$$

so we can deal formally with the I_i' as generators of a rotation group. In order to express $\frac{1}{2}r^2$ as a lowering operator in $SU(2)$ we rotate the generators by $\pi/2$ around the axis 1, i.e.

$$I_1'' = I_1', \quad I_2'' = I_3', \quad I_3'' = -I_2', \tag{4.9}$$

and thus

$$\tfrac{1}{2}r^2 = I_3' + iI_1' = i(I_1'' - iI_2''). \tag{4.10}$$

As the rank 1 irreducible tensors in $SU(2)$ are

$$I_{\pm1}'' = \mp (2)^{-1/2}(I_1'' \pm iI_2''), \quad I_0 = I_3'', \tag{4.11}$$

we can build the rank k and projection $-k$ irreducible tensor in the I_i'' as

$$(\tfrac{1}{2}r^2)^k = i^k(I_1'' - iI_2'')^k = i^k 2^{k/2}(I_{-1}'')^k \equiv i^k 2^{k/2}\mathcal{T}_{-k}^k(I''). \tag{4.12}$$

We can now express r^{2k} in terms of I' undoing (4.9) through the rotation matrices $\mathfrak{D}_{mm'}^f(\alpha\beta\gamma)$, i.e.,[16]

$$\begin{aligned}(\tfrac{1}{2}r^2)^k &= i^k 2^{k/2}\sum_\tau \mathcal{T}_\tau^k(I')\mathfrak{D}_{\tau,-k}^k(\pi/2,\pi/2,-\pi/2)\\ &= \sum_\tau (-i)^\tau 2^{-k/2}[(2k)!]^{1/2}\\ &\quad\times[(k+\tau)!(k-\tau)!]^{-1/2}\mathcal{T}_\tau^k(I').\end{aligned} \tag{4.13}$$

Now in order to pass from the $SU(2)$ irreducible tensors $\mathcal{T}_\tau^k(I')$ of (4.13), to the $SU(1,1)$ irreducible tensors $\mathcal{T}_\tau^k(I)$, we notice that the former are defined by

$$SU(2)\begin{cases} I_\pm' = I_1' \pm iI_2', & [I_\pm', \mathcal{T}_\tau^k(I')] = [(k\mp\tau)(k\pm\tau+1)]^{1/2}\mathcal{T}_{\tau\pm1}^k(I')\\ I_0' = I_3', & [I_0', \mathcal{T}_\tau^k(I')] = \tau\mathcal{T}_\tau^k(I'),\end{cases} \tag{4.14}$$

while the latter are characterized by[12,15]

$$SU(1,1)\begin{cases} I_\pm = I_1 \pm iI_2, & [I_\pm, \mathcal{T}_\tau^k(I)] = \pm[(k\mp\tau)(k\pm\tau+1)]^{1/2}\mathcal{T}_{\tau\pm1}^k(I)\\ I_0 = I_3, & [I_0, \mathcal{T}_\tau^k(I)] = \tau\mathcal{T}_\tau^k(I).\end{cases} \tag{4.15}$$

From these relations and (4.7) we see that

$$\mathcal{T}_\tau^k(I') = i^\tau\mathcal{T}_\tau^k(I). \tag{4.16}$$

Carrying the corresponding substitution in (4.13), we finally obtain, using the Wigner–Eckart theorem,

$$\begin{aligned}I_{n'n}^{k\mu} &\equiv \int_0^\infty f_{n'}^\mu(r)(\tfrac{1}{2}r^2)^k f_n^\mu(r)dr\\ &= \sum_\tau\left[\left(\frac{(k!)^2}{(k+\tau)!(k-\tau)!}\right)^{1/2}\frac{\langle\mu,n,k,\tau|\mu,n'\rangle_{\text{n.c.}}}{\langle\mu,0,k,0|\mu,0\rangle_{\text{n.c.}}}\right]\\ &\quad\times\int_0^\infty f_0^\mu(r)(\tfrac{1}{2}r^2)^k f_0^\mu(r)dr.\end{aligned} \tag{4.17}$$

The brackets $\langle|\rangle_{\text{n.c.}}$ stand for the Wigner coefficients of the noncompact group $SU(1,1)$. These coefficients were given by Ui[15] for integer μ; but this formula is still valid for arbitrary μ. As the last integral is trivial to determine, we get from the explicit expression of $\langle|\rangle_{\text{n.c.}}$, and the selection rule[15] $n+\tau=n'$,

$$I^{k\mu}_{n'n} = \frac{(-1)^{n+n'}}{2^k} \frac{k!\,\Gamma(k+\mu+1)}{(k+n'-n)!} \left(\frac{n!\,n'!\,\Gamma(n'+\mu+1)}{\Gamma(n+\mu+1)}\right)^{1/2} \times \sum_{p=\max(0,n-n')}^{\min(n,k+n-n')} \left(\frac{(k+n'-n+p)!}{p!(k+n-n'-p)!(n-p)!(n'-n+p)!\,\Gamma(n'-n+\mu+p+1)}\right). \quad (4.18)$$

The relation $-k \leq \tau \leq k$ implies the selection rule $|n-n'| \leq k$.

B. Matrix Elements of ρ^k for the Pseudo-Coulomb Problem

For the pseudo-Coulomb problem we need to calculate the matrix elements

$$\int_0^\infty F^{\rm M}_n(\rho)\rho^k F^{\rm M}_{n'}(\rho)\rho^{-1}d\rho, \quad (4.19)$$

as we are using the normalization condition (3.8). Taking then (3.22a) and (3.31) into account, we immediately see that the integral is identical to (4.17) and thus is given by the $I^{k2{\rm M}}_{n'n}$ of (4.18).

C. Matrix Elements of r^k for the Coulomb Problem

For the Coulomb problem the states are normalized according to (3.7) and thus we are interested in the integral

$$J^{k{\rm M}}_{nn'} \equiv (A^c_{n{\rm M}}/A^p_{n{\rm M}})(A^c_{n'{\rm M}}/A^p_{n'{\rm M}}) \int_0^\infty F^M_n(r/\nu)r^k F^M_{n'}(r/\nu')dr, \quad (4.20)$$

where A^c_{nl}, A^p_{nl} are given by (3.7b) and (3.8b), respectively, and ν, ν' and n, n' are related by (3.5). As before the functions $F^{\rm M}_n(\rho)$ are normalized in the sense (3.8). Introducing then the variable $\rho = (r/\nu)$, we can write

$$J^{k{\rm M}}_{nn'} = [nn'(n+{\rm M}+\tfrac{1}{2})(n'+M+\tfrac{1}{2})]^{-1/2} \times \nu^{k+1} \int_0^\infty F^{\rm M}_n(\rho)\rho^{k+1}F^{\rm M}_{n'}(\nu\rho/\nu')\rho^{-1}d\rho. \quad (4.21)$$

From (2.17) we easily see that

$$\lim_{\substack{b\to 0\\ d=a^{-1}}} \langle r'|U_\mu|r''\rangle = i^{-\mu-1}a^{-1/2}\delta(r'-a^{-1}r''), \quad (4.22)$$

and thus using (3.32) we obtain

$$F^{\rm M}_{n'}(\nu\rho/\nu') = \sum_{n''} (\nu/\nu')^{1/2} F^{\rm M}_{n''}(\rho) i^{\mu+1} \times \langle n''|U_{2M}|n'\rangle_{\alpha=0,\beta=\ln(\nu/\nu'),\gamma=0}, \quad (4.23)$$

where the matrix element is given by (2.25). Combining the previous results, we obtain

$$J^{k{\rm M}}_{nn'} = [nn'(n+{\rm M}+\tfrac{1}{2})(n'+{\rm M}+\tfrac{1}{2})]^{-1/2}(\nu/\nu')^{1/2} i^{\mu+1} \times \sum_{n''} \{I^{k2M}_{nn''}\langle n''|U_{2M}|n'\rangle_{\alpha=0,\beta=\ln(\nu/\nu'),\gamma=0}\}, \quad (4.24)$$

where, because $|n-n''| \leq k$, the summation is a finite one.

We have thus achieved by group theoretical means the determination of the radial integrals in the pseudo-Coulomb and Coulomb problems. We note though that we have the same M in both radial wavefunctions. This is unavoidable if we consider the radial problem as one-dimensional, forgetting its relations with other coordinates in a higher-dimensional space in which it can be embedded. If we think in terms of the groups of canonical transformations in these higher-dimensional spaces, we can obtain matrix elements for different irreducible representations of $SU(1,1)$ in bra and ket as was shown for the oscillator case in Ref. 12.

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