Coulomb wave functions in the $\vec{u}$ representation

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A new transformation for the Coulomb problem is introduced and its significance is discussed. Coulomb wave functions in the $\vec{u}$ representation are derived. Examples of the application of the transformation are given.

I. INTRODUCTION

The Coulomb system has been a problem of interest to physicists and mathematicians for many decades. Among the works published, the review articles by Bander and Itzykson[1] and the monograph by Englefield[2] dealt with the symmetry aspects of the problem. On the other hand, Chen and Chen[3] gave a comprehensive account of the two-body Coulomb amplitudes. A recent article by Abarbanel[4] on the "inverse r-squared force" confirms the sustained interest in the problem.

More recently, we discovered a new self-adjoint operator $\vec{A}_0$ and used it to derive a differential equation for the zero-energy wave function in the $\vec{u}$ representation,[5] which has been obtained hitherto by solving an integral equation. This discovery has made possible a transformation from the set of dynamical variables $\vec{r}$ and $\vec{p}$ to the new set $\vec{u}$ and $\vec{A}_0$, and hence a new way of geometrizing the Coulomb field.[6] The new way, as we shall see, is a more appropriate way for the problem at hand.

In Sec. II, we will introduce the new transformation. We will then discuss the geometrical and physical significance of the new transformation in Sec. III. In Sec. IV, we will generalize our previously obtained zero-energy result to wave functions for nonzero energies. Section V contains some possible applications of the transformation. Finally, in Sec. VI, we will make some concluding remarks.

II. TRANSFORMATION

The work of Pauli,[7] Fock,[8] and Bargmann[9] sought to explain the additional degeneracy of the nonrelativistic hydrogen atom in terms of the symmetry group of the four-dimensional rotations in projective momentum space. Accordingly, a point in momentum space is projected stereographically onto a unit hypersphere in a four-dimensional space with the use of Fock coordinates

$$\vec{\xi} = 2p_0\vec{p}/(p^2+p_0^2), \quad \xi_0 = (p^2-p_0^2)/(p^2+p_0^2), \tag{1}$$

where $p_0^2 = -2\mu E$.

The new transformation is based upon the introduction of the following operators:

$$\vec{u} = 2p_c\vec{p}/p^2, \tag{2}$$

$$\vec{A}_0 = -(\vec{r}p^2 + p^2\vec{r})/4p_c + [\vec{p}(\vec{p}\cdot\vec{r}) + (\vec{r}\cdot\vec{p})\vec{p}]/2p_c, \tag{3}$$

$$\vec{B} = \vec{A}_0 + i\hbar\vec{u}/u^2, \tag{4}$$

$$\vec{r} = -(\vec{A}_0u^2 + u^2\vec{A}_0)/4p_c + [\vec{u}(\vec{A}_0\cdot\vec{u}) + (\vec{u}\cdot\vec{A}_0)\vec{u}]/2p_c, \tag{5}$$

where $p_c = Ze^2\mu$ is taken to be positive for an attractive Coulomb potential. The operators $\vec{u}$ and $\vec{A}_0$ satisfy the canonical commutation relations

$$[A_{0\alpha}, A_{0\beta}] = 0, \quad [u_\alpha, A_{0\beta}] = i\hbar\delta_{\alpha\beta}. \tag{6}$$

Consequently, $\vec{A}_0$ admits the operator representation

$$\vec{A}_0 = -i\hbar\vec{\nabla}_u. \tag{7}$$

We have already used this to derive a differential equation for the zero-energy hydrogen wave function in the $\vec{u}$ representation. The solution thus obtained is in agreement with the result obtained by solving an integral equation.[10]

III. SIGNIFICANCE OF THE TRANSFORMATION

To see further what is so good about this transformation, let us observe (a) the zero-energy behavior of the Casimir operator of the degeneracy group $SO(4)$, (b) the line element in Einstein spaces, and (c) the classical trajectories in the $\vec{u}$ space.

A. Casimir operator

In accordance with the new transformation, we introduce the new Fock coordinates

$$\vec{\xi} = 4\nu\vec{u}/(4\nu^2+u^2), \quad \xi_0 = (4\nu^2-u^2)/(4\nu^2+u^2), \tag{8}$$

where $\nu = p_c/p_0$. In spherical polar coordinates, we have for the Fock coordinates

$$\xi = (\sin\alpha\sin\theta\cos\phi, \sin\alpha\sin\theta\sin\phi, \sin\alpha\cos\theta, \cos\alpha) \tag{9}$$

and for the Casimir operator[11]

$$C = -\partial^2/\partial\alpha^2 - 2\cot\alpha(\partial/\partial\alpha) + L^2/\hbar^2. \tag{10}$$

Accordingly, we obtain the Casimir operator in the $\vec{u}$ representation

$$C(u) = -\frac{(4\nu^2+u^2)^2}{16\nu^2}\frac{d^2}{du^2} - \frac{(4\nu^2+u^2)}{2u}\frac{d}{du} + \frac{(4\nu^2+u^2)^2}{16\nu^2u^2}L^2 . \quad (11)$$

Taking the zero-energy limit, which is tantamount to contracting $SO(4)$ to $E(3)$, we obtain

$$C_0(u) = \lim_{\nu\to\infty}\frac{C(u)}{\nu^2} = -\frac{d^2}{du^2} - \frac{2}{u}\frac{d}{du} + \frac{L^2}{u^2} . \quad (12)$$

It follows naturally that the zero-energy partial-wave solution $j_l(u)$ satisfies

$$C_0(u)\, j_l(u) = j_l(u) , \quad (13)$$

which is indeed the equation for spherical Bessel functions. On the other hand, the Casimir operator in the $\vec{p}$ representation

$$C(p) = -\frac{(p_0^2+p^2)^2}{4p_0^2}\frac{d^2}{dp^2} - \frac{(p_0^2+p^2)}{2p}\frac{d}{dp} + \frac{(p_0^2+p^2)^2}{4p_0^2p^2}L^2 \quad (14)$$

yields the zero-energy limit

$$C_0(p) = \lim_{p_0\to 0} 4p_0^2 C(p) = -p^4\left(\frac{d^2}{dp^2} - \frac{L^2}{p^2}\right) . \quad (15)$$

Though the zero-energy partial-wave solution $j_l(2p_c/p)$ does satisfy the equation

$$C_0(p)\, j_l(2p_c/p) = j_l(2p_c/p) , \quad (16)$$

the equation takes on the bona fide form of an equation for spherical Bessel functions only when the transformation $p = 2p_c/u$ is made in accordance with Eq. (2). This supports our contention that the $\vec{u}$ representation is the proper representation for the Coulomb problem of all energies.

B. Line element

The Fock coordinates defined in Eq. (1) or Eq. (8) can both be considered as parametric representation of a hypersphere

$$R_0^2\vec{\xi}^2 + R_0^2\xi_0^2 = R_0^2 \quad (17)$$

of radius $R_0 = p_0$ or $R_0 = \nu$ in a four-dimensional space according to whether the components of $\vec{p}$ or $\vec{u}$ are taken as parameters. In other words, both stereographic projections put the group manifold in the interior of a three-dimensional sphere of radius R_0. However, the line elements of the two hypersurfaces given by

$$ds^2 = 4\,dp^2/(1+p^2/p_0^2)^2 \quad (18)$$

and

$$ds^2 = du^2/(1+u^2/4\nu^2)^2 \quad (19)$$

lead to vastly different geometrical and physical consequences. The line element given by Eq. (19) on hypersurfaces of fixed energy represents a line element in Einstein spaces of constant curvature.[12] It has a well-defined nonvanishing zero-energy limit as $R_0 = \nu \to \infty$. It should be noted that our zero-energy limit happens to be the noncosmological limit.[13] Furthermore, Eq. (19) is in the form of a line element along the optical path in a medium of index of refraction

$$n(u) = 1/(1+u^2/4\nu^2) , \quad (20)$$

which tends to unity as ν tends to infinity. Therefore, in terms of $n(u)$, the Coulomb problem can be properly related by optical-mechanical analogy to the Maxwell fish-eye problem,[14,15] for which the index of refraction

$$n(r) = 1/(1+r^2/R_0^2) \quad (21)$$

approaches unity as $R_0 \to \infty$ as in the case of $n(u)$. Clearly, the line element given by Eq. (18) does not have these properties.

C. Classical trajectories

The classical correspondence of the quantum-mechanical Coulomb problem has been discussed by Gutzwiller[16] and Norcliffe *et al.*[17] in terms of momentum space trajectories, known as hodographs. For the attractive Coulomb potential, the momentum-space trajectories are given by

$$p_x^2 + (p_y - \epsilon p_c/L)^2 = (p_c/L)^2 , \quad (22)$$

where $\epsilon = (1+2mEL^2/p_c^2)^{1/2}$ is the eccentricity of classical orbits. Equation (22) represents a circle with its center on the positive p_y axis and an energy-independent radius p_c/L. As the energy increases, the center moves away from the origin. At $E=0$, all trajectories corresponding to different angular momenta are tangent to each other at the origin. For a repulsive potential $p_c \to -p_c$, we have

$$p_x^2 + (p_y + \epsilon p_c/L)^2 = (p_c/L)^2 . \quad (23)$$

Hence the center of the circular trajectories is located on the negative p_y axis instead. It should be noted that Eq. (23) for the repulsive case can be obtained from Eq. (22) for the attractive case by making an inversion $\vec{p} \to (p_0^2/p^2)\vec{p}$.

The trajectories in the $\vec{u}$ space are given by

$$u_x^2 + (u_y + 2\epsilon\nu^2/L)^2 = (2\nu^2/L)^2 , \quad (24)$$

which is invariant with respect to the sign of the Coulomb potential. The + and − signs are for $E<0$ and $E>0$, respectively. Therefore, the centers of trajectories for positive and negative energies are located on the positive and negative u_y axis, re-

spectively. As E increases, the centers recede away from the origin. For $E=0$, we have $u_y=L$. Therefore, there is no accumulation point for the "angular momentum" trajectories for various angular momenta in the $\vec{u}$ space as in the $\vec{p}$ space. Furthermore, the fact that Eq. (24) is invariant with respect to the sign of the potential suggests that the inaccessible region of one is the analytical continuation of the accessible region of the other.

IV. DERIVATION OF WAVE FUNCTIONS

Having introduced the transformation and discussed its significance, we now proceed to derive the Coulomb wave functions for nonzero energies in the $\vec{u}$ representation. To do so, we begin with the Schrödinger equation for negative energies

$$(p^2/2\mu - Ze^2/r)\Phi = -(p_0^2/2\mu)\Phi . \tag{25}$$

Using the relations

$$B = rp^2/2p_c , \tag{26}$$

$$r = Bu^2/2p_c , \tag{27}$$

which can be obtained from Eqs. (4) and (5), respectively, we can transform Eq. (25) into

$$B(1+u^2/4\nu^2)\Phi = \Phi . \tag{28}$$

We now introduce a unit vector $\vec{\lambda}$ and rewrite Eq. (28) in the form

$$\vec{B}(1+u^2/4\nu^2)\Phi(\vec{u}) = \vec{\lambda}\Phi(\vec{u}) . \tag{29}$$

Since $\vec{B}$ admits, according to Eqs. (4) and (7), the operator representation

$$\vec{B} = -i\hbar u \vec{\nabla}_u u^{-1} , \tag{30}$$

we have finally from Eq. (29)

$$-i\hbar\vec{\nabla}_u(1+u^2/4\nu^2)\Psi(\vec{u}) = \vec{\lambda}\Psi(\vec{u}) , \tag{31}$$

where we have made the substitution

$$\Phi(\vec{u}) = u\Psi(\vec{u}) . \tag{32}$$

Equation (31) can be solved[18] to give the eigenfunction associated with the Hermitian operator $\vec{A}_0$ and normalized on the energy scale

$$\Psi(\vec{u}) = \frac{(2\mu)^{1/2}\nu^2}{p_c(4\nu^2+u^2)} \exp\left[-\frac{2i\nu\vec{\lambda}\cdot\vec{u}}{\hbar u}\tan^{-1}\left(\frac{u}{2\nu}\right)\right]. \tag{33}$$

It can easily be verified that the wave function has the correct zero-energy limit[19]

$$\Psi_0(\vec{u}) = \lim_{\nu\to\infty}\Psi(\vec{u}) = \text{const}\times\exp(i\vec{\lambda}\cdot\vec{u}/\hbar) , \tag{34}$$

a partial-wave expansion of which yields the partial-wave solution $j_l(u)$ in Eq. (13). The solution for positive energies can be obtained in a similar manner. It should be noted that the requirement of single valuedness of the solution given by Eq. (33) yields the well-known bound-state energies $E_n = -Z^2e^4m/2n^2\hbar^2$. The momentum space wave functions are related to our solution by

$$\Psi(\vec{p}) = \Psi(\vec{u})/p^4 , \tag{35}$$

where $\vec{u}$ is given in Eq. (2).

V. APPLICATIONS

While the full implication of the new transformation is yet to be explored, in this section we present some results as examples of its possible application.

A. Overlap integral

The overlap of the radial wave functions R_n and R_0 does not seem to vanish and to be readily calculable. However, we can easily calculate the overlap integral of $\Psi(\vec{u})$ and $\Psi_0(\vec{u})$ and obtain the following result from Eqs. (33) and (34)

$$\int_0^\infty \Psi(\vec{u})\Psi_0(\vec{u})\,d\vec{u} = (\mu/\pi)^{1/2}\hbar\nu^2/2p_c . \tag{36}$$

The angular part of the integral can easily be carried out. By letting $y = u - 2\nu\arctan(u/2\nu)$ and noting $\int_0^\infty dy\,\sin cy/y = \frac{1}{2}\pi\,\mathrm{sgn}(c)$, the above result can be verified. The implications and usefulness of this result have yet to be investigated. As ν tends to infinity, $\sin y/y$ in the integrand tends to unity and Eq. (36) becomes, except for a constant factor, the normalization integral for $\Psi_0(\vec{u})$.

B. Matrix element of the dipole operator

The matrix element of the dipole operator $\vec{r}$ has been evaluated[20] by Barut and Kleinert in terms of a dilatation operator and a fiber space of the hydrogenic wave functions. We show in this subsection how this result can be obtained by using the newly identified operator[21] $\vec{B}$, which is related to the Runge-Lenz vector $\vec{A}$ as follows[5]:

$$\vec{B} = \vec{A} + \mu\vec{r}H/p_c . \tag{37}$$

Since $[\vec{A}, H] = 0$ and $[\vec{r}, H] = i\hbar\vec{p}/\mu$, we have from Eq. (37)

$$[\vec{B}, H] = i\hbar\vec{p}H/p_c . \tag{38}$$

Taking matrix elements of the above two equations between hydrogenic wave functions and combining the results, we obtain

$$\langle nlm|\vec{r}|n'l'm'\rangle = \frac{i\hbar}{\mu(E_{n'}-E_n)}\langle nlm|\vec{p}|n'l'm'\rangle - \frac{p_c}{\mu E_{n'}}\langle nlm|\vec{A}|n'l'm'\rangle . \tag{39}$$

In terms of the generators of the dynamical group for the hydrogen atom (see Appendix), we can show directly[22]

$$nn'\langle nlm|\vec{p}|n'l'm'\rangle = \langle nlm|\exp(-i\theta_{nn'}T)\vec{\Gamma}|n'l'm'\rangle . \tag{40}$$

Substitution of Eq. (40) into Eq. (39) yields the well-known result[20,22]

$$\langle nlm|\vec{r}|n'l'm'\rangle = \frac{i\hbar}{\mu\omega_{nn'}nn'}\langle nlm|\exp(-i\theta_{nn'}T)\vec{\Gamma}|n'l'm'\rangle + \frac{2\hbar^2n^2}{p_c}\langle nlm|\vec{A}|n'l'm'\rangle , \tag{41}$$

where

$$\omega_{nn'} = E_{n'} - E_n = (p_c^2/2\mu\hbar^2)(n'^2 - n^2)/n^2n'^2 .$$

Thus it is seen that, while the Hermitian operator $\vec{A}$ generates $n = n'$ transitions, the non-Hermitian operator $\vec{B}$ generates $n \neq n'$ transitions.

C. Symmetry between attractive and repulsive cases ($E > 0$)

In this subsection, we establish the symmetry relation

$$\langle\Psi_f|O^n|\Psi_i\rangle_{\text{att}} = \exp[\pi(\nu_f - \nu_i)]\langle\Psi_f|O^n|\Psi_i\rangle_{\text{rep}} , \tag{42}$$

where the observable O stands for r, p, $\vec{r}$ or $\vec{p}$. Such symmetry relations have been demonstrated and discussed by Biedenharn *et al.*[23] in connection with the radiative properties of charge particles moving in attractive and repulsive Coulomb fields in terms of a classical contour integration and Sommerfeld's integral. We will establish the symmetry relation Eq. (42) in terms of the properties of the dynamical group for the hydrogen atom.

To begin with, we consider

$$\langle\Psi_f|O|\Psi_i\rangle_{\text{att}} = \int d\vec{p}\,\Psi_f^*(\vec{p})O\Psi_i(\vec{p}) , \tag{43}$$

$$\langle\Psi_f|O|\Psi_i\rangle_{\text{rep}} = \int d\vec{p}'\,\Psi_f^*(\vec{p}')O\Psi_i(\vec{p}') , \tag{44}$$

where the subscripts stand for the set νlm and[24]

$$\vec{p}' = (p_0^2/p^2)\vec{p} . \tag{45}$$

Both of the wave functions $\Psi(\vec{p})$ and $\Psi(\vec{p}')$ satisfy the integral equation for $p_0^2 = 2\mu E$

$$(q^2 - p_0^2)\Psi(\vec{q}) - \frac{Ze^2}{2\pi^2}\int\frac{d\vec{q}'\Psi(\vec{q}')}{|\vec{q}' - \vec{q}|^2} = 0 . \tag{46}$$

Note, however, that the substitution of $\Psi(\vec{p}')$ into Eq. (46) results in a change of the sign of the integral. This sign change, tantamount to the change $-e$ to e, makes $\Psi(\vec{p})$ and $\Psi(\vec{p}')$ the wave functions for attractive and repulsive potentials, respectively.

Noting that Eqs. (2) and (45) give $\vec{p}' = \vec{u}/2a$ where $a = p_c/p_0^2$, we now transform $\Psi(\vec{p}')$ into the $\vec{u}$ representation by making use of the unitary scaling operator $S(\beta)$, $\beta = 1/2a$, which has these pertinent properties[25]:

$$S(\beta)\Psi(\vec{p}) = \beta^{3/2}\Psi(\beta\vec{p}) ,$$

$$S(\beta)O^n = \beta^n O^n S(\beta) ,$$

$$S^*(\beta) = S(1/\beta) .$$

Consequently, Eq. (44) becomes

$$\langle\Psi_f|O|\Psi_i\rangle_{\text{rep}} = 2a\int\Psi_f^*(\vec{u})O\Psi_i(\vec{u})d\vec{u} . \tag{47}$$

We now express the integrals in Eqs. (43) and (47) as invariant matrix elements[26] of $\vec{\rho}O$ and $\vec{\rho}'O$, where (see Appendix)

$$\vec{\rho} = (\vec{\Gamma}_0 - \vec{S})/p_0 , \tag{48}$$

$$\vec{\rho}' = (\vec{\Gamma}_0 - \vec{S})/2\nu , \tag{49}$$

between the tilted states in the $\vec{p}$ and $\vec{u}$ representations

$$\bar{\Phi}_{\nu lm}(\xi) = (p^2 - p_0^2)^2\Psi_{\nu lm}(\vec{p})/4p_0^2 , \tag{50}$$

$$\bar{\Phi}_{\nu lm}(\xi') = (u^2 - 4\nu^2)^2\Psi_{\nu lm}(\vec{u})/16\nu^2 , \tag{51}$$

where ξ and ξ' are given by Eqs. (1) and (8), respectively, except with + and − signs interchanged. Accordingly, we have

$$\langle\Psi_f|O|\Psi_i\rangle_{\text{att}} = \int\bar{\Phi}_f^*(\xi)\vec{\rho}O\bar{\Phi}_i(\xi)d\Omega_\xi , \tag{52}$$

$$\langle\Psi_f|O|\Psi_i\rangle_{\text{rep}} = 2a\int\bar{\Phi}_f^*(\xi')\vec{\rho}'O\bar{\Phi}_i(\xi')d\Omega_{\xi'} , \tag{53}$$

where

$$d\Omega_\xi = (2p_0)^3d^3p/(p^2 - p_0^2)^3 , \tag{54}$$

$$d\Omega_{\xi'} = (4\nu)^3d^3u/(u^2 - 4\nu^2)^3 . \tag{55}$$

Since ξ and ξ' are points on different sheets of the hyperbloid $\xi_0^2 - \vec{\xi}^2 = 1$, we have[1]

$$\bar{\Phi}_f^*(\xi') = \exp(\pi\nu_f)\bar{\Phi}_f^*(\xi) , \tag{56}$$

$$\bar{\Phi}_i(\xi') = \exp(-\pi\nu_i)\bar{\Phi}_i(\xi) . \tag{57}$$

Furthermore, it can easily be shown that

$$\vec{\rho} = 2a\vec{\rho}' , \tag{58}$$

$$\int d\Omega_\xi = \int d\Omega_{\xi'} . \tag{59}$$

Combining Eqs. (52) to (59), we obtain the desired result

$$\langle\Psi_f|O|\Psi_i\rangle_{\text{att}} = \exp\pi(\nu_f - \nu_i)\langle\Psi_f|O|\Psi_i\rangle_{\text{rep}} . \tag{60}$$

In a similar manner, the symmetry relation Eq. (42) can be established by replacing O^n by $(\vec{p}O)^n$

VI. CONCLUDING REMARKS

We have introduced the new transformation for the Coulomb problem and discussed its significance. We have also given some examples of its possible application. The usefulness and implications of the new transformation needs to be further explored.

APPENDIX: PHYSICAL REALIZATIONS OF THE $SO(4,2)$ GENERATORS

The 15 generators of the dynamical group for the hydrogen atom admit the following realizations in the $\vec{p}$ and $\vec{u}$ representations:

$$\vec{L}=\vec{r}\times\vec{p}=\vec{u}\times\vec{B} \text{ or } \vec{u}\times\vec{A}_0,$$

$$-\vec{A}=-\vec{B}-\vec{r}/2a,$$

$$\vec{M}=-\vec{B}+\vec{r}/2a,$$

$$\vec{\Gamma}=r\vec{p}/\nu=B\vec{u}/\nu,$$

$$\Gamma_0=\tfrac{1}{2}(rp^2/p_c+r/a)=B+Bu^2/4\nu^2,$$

$$S=\tfrac{1}{2}(rp^2/p_c-r/a)=B-Bu^2/4\nu^2,$$

$$T=i\hbar(\vec{r}\cdot\vec{p}-i\hbar)/\nu^2$$
$$=i\hbar(\vec{u}\cdot\vec{B}-2i\hbar)/\nu^2 \text{ or } i\hbar(\vec{u}\cdot\vec{A}_0-i\hbar)/\nu^2,$$

where

$$\vec{B}=-\vec{r}p^2/2p_c+\vec{p}(\vec{r}\cdot\vec{p})/p_c,$$

$$\vec{r}=-\vec{B}u^2/2p_c+\vec{u}(\vec{B}\cdot\vec{u})/p_c.$$

The newly identified operator $\vec{B}$ is therefore given by

$$\vec{B}=\tfrac{1}{2}(\vec{A}-\vec{M}).$$

It should be noted that by setting $p_c=a=\hbar=\nu=1$, the generators in the $\vec{p}$ representation take the forms given by Barut and Bronzin.[27] It should also be noted that in the $\vec{u}$ representation the non-Hermitian operator $\vec{B}$ instead of the Hermitian operator $\vec{A}_0$ plays the central role. The operators $\vec{B}$ and $\vec{A}_0$ satisfy the same commutation relations with $\vec{u}$.[5] In the zero-energy limit, $\nu\to\infty$, we have from the $\vec{u}$ representation

$$\vec{L}=\vec{r}\times\vec{B},\quad \vec{A}=\vec{B},\quad \vec{M}=-\vec{B},$$

$$\vec{\Gamma}=0,\quad \Gamma_0=B,\quad S=B,\quad T=0.$$

The significance and the implications of the above dual realization are being investigated.[28]

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