Dynamic algebras of the two-center Coulomb problem

A. M. Frolov
I. V. Kurchatov Institute of Atomic Energy, Moscow

(Submitted 21 July 1983)
Pis'ma Zh. Eksp. Teor. Fiz. **38**, No. 10, 501–505 (25 November 1983)

Dynamic algebras are derived for the two-center Coulomb problem. The representations of these algebras are examined. The conditions under which the representations of these dynamic algebras are equivalent are derived. This new approach is useful for determining the analytic properties of the two-center Coulomb wave functions, for finding the recurrence relations among the integrals of these functions, etc.

PACS numbers: 03.65.Fd

The successful use of representations of the groups[1,2] $O(2,2)\otimes O(4)$ and $O(2,2)\otimes O(2,2)$ in the two-center Coulomb problem has pointed out the need to construct dynamic groups for systems of this type. In the present letter we derive the corresponding algebras; for the representations we find the conditions for equivalence of the initial two-center Coulomb problems, on the one hand, and the single-center Coulomb problems, on the other.

We consider the nonrelativistic Coulomb problem of two fixed centers q_1 and $q_2(|q_1|\geqslant|q_2|)$. These centers lie on the z axis and are separated by a distance R; the origin of coordinates is at the center at the left. We use atomic units. We adopt the prolate spheroidal coordinates ξ, η, α, which are related to the Cartesian coordinates by

$$x = \frac{R}{2}\sqrt{(\xi^2-1)(1-\eta^2)}\cos\alpha\,; \quad y = \frac{R}{2}\sqrt{(\xi^2-1)(1-\eta^2)}\sin\alpha\,,$$
$$z = \frac{R}{2}(\xi\eta+1)\,. \tag{1}$$

The variables ξ, η, α can be separated in the Schrödinger equation, and the wave function $\psi_i(\xi,\eta,\alpha;R)$ can be written

$$\psi_j(\xi,\eta,\alpha;R) = N_j(R)\,\Pi_j^1(\xi,R)\,\Sigma_j^1(\eta,R)\,e^{im\alpha}\,. \tag{2}$$

As an example, the equation for the function $\pi_j^1(\xi,R)$ is[3]

$$\left[\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi} + \frac{R^2}{2}E_j(\xi^2-1) + R(q_1+q_2)\xi + \lambda_j - \frac{m^2}{\xi^2-1}\right]\Pi_j^1(\xi,R) = 0,$$

where $E_j(R)$ is the energy of the system and $\lambda_j(R)$ is a separation constant.

We know that for the same values of R, E, λ, and m^2 there exist solutions of the two-center Coulomb problem for the q_1; $-q_2$ system:

$$\varphi_j(\xi, \eta, a; R) = M_j(R)\, \Pi_j^2(\xi, R)\, \Sigma_j^2(\eta, R)\, e^{im\alpha}, \qquad (2')$$

where $N_j(R)$ and $M_j(R)$ are normalization "constants."

The function $\pi_j^1(\xi, R)$ is the radial Coulomb spheroidal function.[3]

The function $\Sigma_j^1(\eta, R)$ is the angular Coulomb spheroidal wave function of the single-center system $Q_- = q_1 - q_2$. The functions $\pi_j^2(\eta, R)$ and $\Sigma_j^2(\xi, R)$ are the angular and radial Coulomb spheroidal functions for the single-center systems Q_+ and Q_-, respectively.

We denote by Φ the basis functions of the space of representations of the algebras which we are deriving. We seek Φ as the product of (2) and (2'), with $\xi = \xi_1$, $\eta = \eta_2$, $\alpha = \alpha_1$, in (2) and $\xi = \xi_2$, $\eta = \eta_1$, $a = a_2$. in (2').

Straightforward but laborious manipulations lead us to a system of equations for Φ:

$$\begin{cases} \frac{R^2}{2}(\xi_1^2 - \eta_1^2)(H(1, Q_+) - E)\Phi = 0 \\ \frac{R^2}{2}(\xi_2^2 - \eta_2^2)(H(2, Q_-) - E)\Phi = 0, \end{cases} \qquad (3)$$

where $H(i, Q)$ is the Hamiltonian of the single-center Coulomb system Q, written in terms of the prolate spheroidal coordinates, for the variables with index "i". If Eqs. (3) are to be equivalent to the original two-center Schrödinger equation, the following conditions must be satisfied for both equations in (3):

(1) The values of E must be equal. (2) The values of m_1^2 and m_2^2 must be equal. (3) The separation constants λ in terms of the prolate spheroidal coordinates must be equal.

The derive all the solutions of the Coulomb two-center problem by this approach we need to consider the following ranges of the variables: $-1 \leqslant \xi < +\infty$; $-1 \leqslant \eta < +\infty$; $0 \leqslant \alpha < 2\pi$.

Under the assumption that ξ and η vary independently, we find from (1) that x and y can take on either real or imaginary values, while z can be only real. It then follows immediately that Eqs. (3) are equivalent to a set of four systems of equations in Cartesian coordinates and that each of the two equations of these systems is an equation for a single-center coordinates ($r^2 = x^2 + y^2 + z^2$) or pseudo-Euclidean coordinates ($r^2 = -x^2 - y^2 + z^2$). Correspondingly, we find the dynamic algebras corresponding to (3):

1) $SO(4,2) \oplus SO(4,2)$; 2) $SO^*(4,2) \oplus SO(4,2)$;

3) $SO(4,2) \oplus SO^*(4,2)$; 4) $SO^*(4,2) \oplus SO^*(4,2)$,

where $SO^*(4,2)$ is the dynamic algebra of the single-center Coulomb pseudo-Euclidean problem,

$$\sqrt{-x^2 - y^2 + z^2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} + \frac{2Q}{\sqrt{-x^2 - y^2 + z^2}} - 2E\right)\Phi = 0.$$

The dynamic algebra $SO(4, 2)$ has the generators[4]

$$\mathbf{J} = \mathbf{r} \times \mathbf{p}; \quad T = \mathbf{r} \cdot \mathbf{p} - i; \quad \Gamma = r\mathbf{p}; \quad \mathbf{A} = \frac{\mathbf{r}}{r} \Gamma_4 - \mathbf{p}(\mathbf{r}, \mathbf{p}),$$

$$\Gamma_0 = \frac{1}{2} r(p^2 + 1); \quad \Gamma_4 = \frac{1}{2} r(p^2 - 1); \quad \mathbf{M} = \frac{\mathbf{r}}{r} \Gamma_0 - \mathbf{p}(\mathbf{r}, \mathbf{p}). \tag{4}$$

For these generators, the following correspondence has been established $(1 \leqslant i \leqslant 3)$:

$$L_{ij} = \epsilon_{ijk} J_k; \quad L_{i4} = A_i; \quad L_{0i} = M_i; \quad L_{i5} = \Gamma_i; \quad L_{05} = \Gamma_0; \quad L_{45} = \Gamma_4; \quad L_{04} = T.$$

The commutation relation is of the standard form:

$$[L_{ik}, L_{lm}] = i(\delta_{il} L_{km} + \delta_{km} L_{il} - \delta_{im} L_{kl} - \delta_{kl} L_{im}). \tag{5}$$

The invariant operators have the numerical values $C_2 = -6$, $C_3 = 0$, $C_4 = 12$. A basis vector of an $SO(4, 2)$ representation is written as a set of three numbers $|\mu j m|$:

$$J_z |\mu j m\rangle = m |\mu j m\rangle \qquad J^2 |\mu j m\rangle = j(j+1) |\mu j m\rangle$$

$$\Gamma_0 |\mu j m\rangle = \mu |\mu j m\rangle \ (E < 0) \quad \Gamma_4 |\mu j m\rangle = \mu |\mu j m\rangle \ (E > 0). \tag{6}$$

The dynmaic algebra SO*(4,2) has the generators Γ_0, Γ_4, T, J_z, M_z, Γ_z, A_z. These generators are the same as the SO(4, 2) generators, except that $p^2 = -p_x^2 - p_y^2 + p_z^2$ and $r^2 = -x^2 - y^2 + z^2$, where $p_l = (-i)(\partial/\partial x_l)(l = 1,2,3)$ The generators J_x, J_y, A_x, A_y, M_x, M_y, Γ_x, Γ_t become

$$J_x = yp_z + zp_y; \qquad A_x = \frac{1}{2} x(p^2 - 1) + p_x(\mathbf{r}, \mathbf{p})$$

$$J_y = -zp_x - xp_z; \qquad A_y = \frac{1}{2} y(p^2 - 1) + p_y(\mathbf{r}, \mathbf{p})$$

$$\Gamma_x = -rp_x; \qquad M_x = \frac{1}{2} x(p^2 + 1) + p_x(\mathbf{r}, \mathbf{p})$$

$$\Gamma_y = -rp_y; \qquad M_y = \frac{1}{2} y(p^2 + 1) + p_y(\mathbf{r}, \mathbf{p}).$$

If we use the same correspondence as for SO(4,2), then commutation relation (5) is not changed, except in the case in which neither of the generators on the left side of (5) belongs to the subalgebra T, Γ_0, Γ_4, J_z, A_z, $M_z \Gamma_z$. On the right side of (5) we would then have $i \to -i$. The invariant operators have the same values as in SO(4,2). A basis vector of a representation of the SO*(4,2) algebra is also specified as the set of three numbers $|\mu jm\rangle$ $(j = -1/2 + i\sigma|$, where σ is real) and again satisfies conditions (6). We then find immediately that a basis vector of a representation of the dynamic algebras of system (3) is specified as the set of six numbers: $|\mu_1 j_1 m_1\rangle |\mu_2 j_2 m_2\rangle$. We denote by ψ a basis vector of a representation of the dynamic algebra of the two-center Coulomb problem, and we seek this vector as the linear combination

$$\psi = \int \int C_1(\lambda, j_1) C_2(\lambda, j_2) |\mu_1 j_1 m_1\rangle |\mu_2 j_2 m_2\rangle dj_1 dj_2.$$

The equality of the values of E and m^2 yields

$$\frac{Q_+^2}{\mu_1^2} = \frac{Q_-^2}{\mu_2^2}; \qquad m_1^2 = m_2^2 = m^2.$$

The variable-separation operator $\hat{\lambda}$ is

$$\hat{\lambda} = J^2 + R\left[\left(\frac{1}{2} - E\right) A_z + \left(\frac{1}{2} + E\right) M_z\right] + \frac{R^2}{2}\left[r(H-E)\right].$$

In the limit $R \to 0$ we find it in terms of parabolic coordinates. In terms of the unknown vectors ψ, the effect of $\hat{\lambda}$ is equivalent to that of the variable-separation operators in prolate spheroidal coordinates ($\hat{\lambda}_{\mathrm{PSC}}$):

$$\hat{\lambda}_{\mathrm{PSC}} = J^2 + \sqrt{-2E}\, RA_z\ (E<0); \quad \hat{\lambda}_{\mathrm{PSC}} = J^2 + \sqrt{2E}\, RM_z\ (E>0).$$

In general, the equations for $C_1(\lambda, j_1)$ and $C_2(\lambda, j_2)$ which follow from the condition that the values of λ are equal in terms of the prolate spheroidal coordinates are integral equations, whose derivation requires the use of recurrence relations for the coefficients of the vector composition of a representation of the $O(2,1)$ group (the main series). In the case of the dynamic algebra SO(4,2) $\oplus$ SO(4,2), the results of Ref. 5 allow us to reduce the problem to a problem of the equality of the eigenvalues of two finite-dimensional matrices ($E<0$) or infinite-dimensional matrices ($E>0$). Since we have $E<0|m|\leqslant j \leqslant n-1$ in the case $E<0$, the dimensionalities of the two finite-dimensional problems, which have equal eigenvalues only at certain values of R, are $\mu_1 - |m|$ and $\mu_2 - |m|$, as was first found by Demkov.[6] The resulting symmetric three-diagonal matrices $\hat{\lambda}$ have the same matrix elements

$$\lambda_{k,k} = j(j+1), \text{ where}: \quad k = j + 1 - |m|,$$

$$\lambda_{k,k+1} = \frac{|Q|}{\mu} R \sqrt{\frac{[(j+1)^2 - m^2][\mu^2 - (j+1)^2]}{4(j+1)^2 - 1}} \quad (E<0),$$

$$\lambda_{k,k+1} = \frac{|Q|}{\mu} R \sqrt{\frac{[(j+1)^2 - m^2][\mu^2 + (j+1)^2]}{4(j+1)^2 - 1}} \quad (E>0).$$

As an example, the result of Ref. 6 for the system $q_1 = 5$, $q_2 = 1$ ($E<0$) is $\lambda = 1/3$, $R = \sqrt{10/3}$.

I wish to expres my gratitude to N. F. Truskova, S. K. Suslov, and Ya. A. Smorodinskiĭ.

[1]N. F. Truskova, Yad. Fiz. **28**, 558 (1978) [Sov. J. Nucl. Phys. **28**, 284 (1978)].
[2]N. F. Truskova, Yad. Fiz. **29**, 243 (1979) [Sov. J. Nucl. Phys. **29**, 122 (1979)].
[3]V. I. Komarov, L. I. Ponomarev, and S. Yu. Slavyanov, Sferoidal'nye i kulonovskie sferoidal'nye funktsii (Spheroidal and Coulomb Spheroidal Functions), Nauka, Moscow, 1976.
[4]A. Borut and R. Ronchko, Theory of Group Representations and Its Applications (Russ. transl. Mir, Moscow, 1980, Vol. 2).

[5]A. F. Nikiforov and S. K. Suslov, Preprint 83, IPM, 1982.
[6]Yu. N. Demkov, Pis'ma Zh. Eksp. Teor. Fiz. **7**, 101 (1968) [JETP Lett. **7**, 76 (1968)].

Translated by Dave Parsons
Edited by S. J. Amoretty