International Journal of Theoretical Physics, Vol. 16, No. 7 (1977), pp. 517–531

Group-Induced Quantization in Central Problems in Mechanics

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Received: 25 *January* 1977

Abstract

For each bounded trajectory of a particle in an arbitrary central field of force there exists a uniformly rotating reference frame in which the trajectory is closed. This circumstance makes it meaningful to introduce a nonconserving analog of the Runge–Lenze vector and to extend the group-theoretical description of the Kepler problem to the general case. In this paper the classical generators obeying the $O(4.2)$-algebra Poisson-bracket relations are given for the mechanical three-dimensional problem with arbitrary centrally symmetrical potential. A quantization is proposed in which one replaces six classical observables selected among the group generators by the operators obeying the corresponding commutation relations instead of postulating the canonical commutation relations.

1. *Introduction*

In our previous paper[1] (Serebrennikov and Shabad, 1973) we considered bounded motion in a three-dimensional mechanical problem with arbitrary central field of force and built a set of generators of infinitesimal canonical transformations from the $O(4)$ Lie algebra.

Among innumerable ways to do so we chose the one that supplied the constructed algebraic quantities with meaningful dynamical information. Our treatment is based on the fact that each trajectory can be made to be closed by the transition to a uniformly rotating reference frame. In this frame a generalized Runge-Lenze vector is meaningful. It becomes uniformly rotating in the rest frame (we call it the "precession vector" here). Its nonconserving components, along with those of the angular momentum, form the $O(4)$ Poisson-bracket Lie algebra. Similar results are achieved in the relativistic case, and for the $SU(3)$ group (Serebrennikov, 1974; Serebrennikov and Shabad, 1976).

In Section 2, after having rewritten from I some necessary results concerning the $O(4)$ classical generators, we show how to choose six independent

[1] Hereafter referred to as I.

observables associated with the $O(4)$ algebra [and with the wider $O(4.2)$ algebra given in Section 5] that parametrize the phase space.

In Sections 3 and 4 we discuss and fulfill a quantization program which, unlike the canonical quantization scheme, makes use of the above six group-associated observables. Within this program one postulates the commutation relations among these basic observables as they are prescribed by their algebraical meaning instead of postulating the canonical commutation relations between the position and momentum variables. Since the classical energy is uniquely expressed in terms of the above variables [namely, in terms of the mutually commuting Casimir invariants of the $SO(4)$ group and its subgroup $SO(3)$] a natural way arises to define the quantum Hamiltonian in agreement with the correspondence principle and the requirement that in the Coulomb case its spectrum should exactly coincide with the usual hydrogen atom spectrum. The peculiarity of the quantization proposed is in its dynamical origin in the sense that the classical observables that are replaced by quantum operators are potential dependent, which is not the case for the canonical quantization.

In Section 5 we give the expressions for the classical generators of the $SO(4.2)$ algebra using the above six observables. This algebra includes the $O(4)$ as its subalgebra. All the generators of the $SO(4.2)$ are given the quantum definitions in accord with the correspondence principle. When doing so one comes upon an interesting prescription for ordering the basic operators within classical functions containing them.

2. *SO(4)-Algebra of Poisson Brackets and Parametrization of the Phase Space*

In I we studied the general central problem with the Hamiltonian function of the form

$$H = p_i^2/2 + V(r) \tag{2.1}$$

where P_i, r_i $(i = 1, 2, 3)$ are canonical variables satisfying the Poisson-bracket relations

$$\{r_i, p_j\} = \delta_{ij}, \qquad \{p_i, p_j\} = \{r_i, r_j\} = 0 \tag{2.2}$$

$p = (\mathbf{p}^2)^{1/2}$, $r = (\mathbf{r}^2)^{1/2}$ and the potential $V(r)$ must be sufficiently attractive to provide the domain of bounded motion.

In I we built the nonconserving analog of the Runge-Lenz vector $\mathbf{A}$ (which we shall from now on call the precession vector):

$$\mathbf{A} = (2G - L^2)^{1/2} \left(\frac{\mathbf{r}}{r} \cos \xi + \frac{\mathbf{r} \times \mathbf{L}}{rL} \sin \xi \right) \tag{2.3}$$

where[2]

$$\xi(r_{\min}, r) = \int_{r_{\min}}^{r} \frac{L - Fr^2}{r} \{2[H - V(r)]r^2 - L^2\}^{-1/2} \, dr = \varphi - Ft \tag{2.4}$$

[2] The square root in the integrand is meant to change its sign in the turning points so that it will be the same as the sign of $(\mathbf{rp})$.

In (2.3) and (2.4) **L** is the orbital momentum:

$$\mathbf{L} = [\mathbf{r} \times \mathbf{p}] \tag{2.5}$$

G is the function of the energy H and the angular momentum squared L^2:

$$G = \frac{1}{2}\left[L + \frac{1}{\pi}\int_{r_{\min}}^{r_{\max}} \left(2[H - V(r)] - \frac{L^2}{r^2}\right)^{1/2} dr\right]^2 \tag{2.6}$$

$$F = -\partial G/\partial L \left(\frac{\partial G}{\partial H}\right)^{-1} \tag{2.7}$$

and $r_{\min}$ and $r_{\max}$ are the turning (perigee and apogee) points of the trajectory with given H and L. In (2.4) φ is obviously the angular position of the particle and t is the time.

The precession vector (2.3)–(2.7) is defined uniquely [up to an arbitrary choice of the phase made in (2.3)] by the conditions that we now shall list. Along with the orbital momentum it satisfies the Poisson-bracket relations of the the $O(4)$ algebra:

$$\{L_i, L_j\} = \epsilon_{ijk} L_k \tag{2.8}$$

$$\{L_i, A_j\} = \epsilon_{ijk} A_k \tag{2.9}$$

$$\{A_i, A_j\} = \epsilon_{ijk} L_k \tag{2.10}$$

It lies in the plane of motion. This fact provides the vanishing of one out of the two Casimir invariants of the $O(4)$

$$G_0 = (\mathbf{AL}) = 0 \tag{2.11}$$

The other Casimir invariant is just (2.6):

$$G = \tfrac{1}{2}(L^2 + A^2), \qquad \{G, L_i\} = \{G, A_i\} = 0 \tag{2.12}$$

It conserves:

$$\{G, H\} = 0 \tag{2.13}$$

which implies via (2.12) and the relation $\{L, H\} = 0$ the conservation of the length of the precession vector. On the other hand its direction is not conserved:

$$\frac{d\mathbf{A}}{dt} = \{\mathbf{A}, H\} = F\frac{\mathbf{L} \times \mathbf{A}}{L} \tag{2.14}$$

and the precession vector rotates with the constant angular velocity $F(H, L)$ (2.7):

$$\mathbf{A} = \mathbf{A}_0 \cos Ft - (\mathbf{A}_0 \times \mathbf{L}/L) \sin Ft \tag{2.15}$$

F is so fixed by (2.7) and (2.6) that the trajectory of the particle is closed in the reference frame, rotating along with **A** around **L**. Indeed, substituting (2.7)

and (2.6) into (2.4) one sees that $\xi(r_{\min}, r_{\max}) = \pi$ and thus the mutual orientation of the vectors **A** and **r** [see (2.3)] repeats itself with the period

$$T = \frac{2\pi}{(2G)^{1/2}} \frac{\partial G}{\partial H} = \int_{r_{\min}}^{r_{\max}} 2r\{2[H - V(r)]r^2 - L^2\}^{-1/2}\, dr \qquad (2.16)$$

equal to the time distance between two successive perihelions on the given trajectory. Note that the disregard of the rotation effect achieved by putting $F = 0$ in (2.4) converts (2.3) into Fradkin's (1967) piecewise conserving Runge–Lenz vector, which we studied earlier (Serebrennikov and Shabad, 1971).

The last property of the precession vector (2.3) is its vanishing for the circular trajectories (Bacry et al., 1966; Serebrennikov and Shabad, 1971) when $r_{\min} = r_{\max}$ and $G = \frac{1}{2}L^2$ from (2.6).

These are the properties that fix the precession vector up to the phase. The phase arbitrariness reduces to different possible choices of the lower integration limit r_1 in (2.4) $r_{\max} \geqslant r_1 \geqslant r_{\min}$. Any admittable choice of it does not affect the important relation (2.6), which expresses inexplicitly the Hamiltonian as a function of L and G. With our choice $r_1 = r_{\min}$ the precession vector becomes parallel to **r** each time the latter points at a perihelion (see Serebrennikov and Shabad, 1976; and Serebrennikov et al., 1975 for discussion of the arbitrary choice of the phase).

The rest of this section is devoted to the parametrization of the phase space in terms of variables associated with the algebraic quantities. The variables to appear generalize the ones known in the Kepler problem (Bacry et al., 1966).

Reversing relations (2.3) one gets

$$\frac{\mathbf{r}}{r} = \frac{\mathbf{A}}{A}\cos\xi - \frac{\mathbf{A}\times L}{AL}\sin\xi \qquad (2.17)$$

$$\frac{\mathbf{p}}{p} = \frac{\mathbf{A}}{A}\cos(\xi + \sigma) - \frac{\mathbf{A}}{A}\times\frac{\mathbf{L}}{L}\sin(\xi + \sigma) \qquad (2.18)$$

Equation (2.18) is obtained by calculating the vector product of equation (2.17) and **L**. In (2.18) σ is the angle between **r** and **P**:

$$\sigma(r) = \arccos\frac{(\mathbf{rp})}{rp} = \arcsin\frac{L}{r[2(H - V)]^{1/2}} \qquad (2.19)$$

Since ξ and σ are periodic functions of time, one may see from (2.17) and (2.18) that the parametrization of the phase space can be achieved if one adds to the five variables L_i, A_i, $\Sigma_{i=1}^{3} A_i L_i = 0$ a sixth one defined modulo the period T (2.16). As such we may take the time $t(r, r_{\min})$ measured beginning with the perigee point and up to the period T:

$$t(r_{\min}, r) = \int_{r_{\min}}^{r} \left(2H - 2V - \frac{L^2}{r^2}\right)^{-1/2} dr \qquad (2.20)$$

or, alternatively, the dimensionless variable

$$\psi = \frac{2\pi}{T} t(r_{\min}, r), \qquad 0 \leqslant \psi \leqslant 2\pi \tag{2.21}$$

defined modulo 2π. A trajectory is fixed if the orbital momentum **L** and the precession vector **A** are given at a time relating to any moment when **r** and **A** are parallel to each other, i.e., $\psi = 0$ (or $\psi = 2\pi n$). Indeed, H is found by inverting (2.6) with the account of (2.12). The initial momentum length is determined as $p_0 = [2H - 2V(r_{\min})]^{1/2} = L/r_{\min}$, $\xi_0 = 0$, $\sigma_0 = \pi/2$ and $\mathbf{r}_0$ and $\mathbf{p}_0$ are given by (2.17) and (2.18).

The sixth variable ψ (2.21) has the following Poisson-bracket relations with the remaining five variables (Serebrennikov et al., 1975):

$$\{L_i, \psi\} = 0 \tag{2.22}$$

$$\{\psi, A_i/A\} = 0 \tag{2.23}$$

$$\{\psi, (2G)^{1/2}\} = 1 \tag{2.24}$$

It follows from this that

$$\{\psi, A_i\} = \left\{\psi, \frac{A_i}{A}(2G - L^2)^{1/2}\right\} = \frac{A_i}{A}\frac{(2G)^{1/2}}{(2G - L^2)^{1/2}} \tag{2.25}$$

The most important thing about the relations (2.22)–(2.25) is that they are potential independent, just as relations (2.8)–(2.13) are. This enables us to extend some results known in the Kepler problem to the general case under consideration. In the paper by Smorodinsky and the present authors (Serebrennikov et al., 1975), using (2.25), we integrate the $O(4)$ algebraic relations up to the global $SO(4)$-group action on the phase space following the treatment of the Kepler problem by Bacry et al. (1966). The classical generators of other algebras [$O(4.1)$, $O(4.2)$, $O(2.1)$] are also based on the use of the variable ψ and its universal commutation relations (2.22)–(2.25). They will be given in Section 5. In the above-mentioned paper by Smorodinsky and us the geometrical sense of ψ was visualized. There we map the phase space onto the group invariant manifold, whereupon the $SO(4.1)$ group acts linearly via the canonical transformations performed by the Dirac brackets. This manifold is a product of two three-dimensional spheres in the mutually orthogonal four-dimensional "momentum" and "position" spaces with alternatable mutually inverse radii. The Dirac-bracket Hamiltonian formalism in this manifold implies that the particle moves along a diametral circle in the sphere, ψ being its angular position. This motion is uniform according to (2.21). The plane of the circle rotates with the constant angular velocity F (2.7).

In the subsequent sections we shall exploit the universality of relations (2.8)–(2.13) and (2.22)–(2.24) for quantization.

3. *Quantization: General Discussion*

Now we are in a position to give a more elaborate description of the quantization procedure outlined in I, making use of the above algebraic results. Generally the transition from the classical to quantum mechanics is performed in three steps.

Step 1. Quantization. This is to select some six ($2N$, where N is the number of the degrees of freedom) independent observables that parametrize the phase space, and replace them by some ("operator") quantities possessing a noncommutative multiplication law that is governed by a numerical parameter h (the Planck constant). This mutliplication law requires that all the results of commutation among these six operators (divided by ih) should, in the $h \to 0$ limit, coincide with the results of the corresponding Poisson-bracket calculations. We shall refer to these six variables as the "basic" observables. Their choice is a matter of convenience or algebraic elegance of the above commutation relations.

Step 2. Specification of Quantum Dynamics. This is to postulate the Hamiltonian as a function of the above six basic operators in such a way that in the $h \to 0$ limit this function should coincide with the classical Hamiltonian when expressed as a function of the corresponding six c-numerical variables and that this operator should be Hermitian.

Step 3. Definition of Various Observables. This is to establish the operator expressions for some important observables (besides the Hamiltonian) so that they could have necessary physical meaning. If an observable must, owing to its physical sense, have a classical analog, the $h \to 0$ limiting process should turn it into the corresponding classical function of the six basic variables. Besides the physical meaning some other, formal prescription may naturally arise within the general algebraic framework which rules the way the six basic operators should be ordered as arguments of the observable and thus define the operator corresponding to it.

Now that we have formulated Steps 1, 2, and 3 we shall describe them for our "algebraic" quantization scheme as compared with the canonical quantization.

Within the usual canonical quantization scheme it is the Euclidean canonically conjugated variables $\mathbf{r}$, $\mathbf{p}$ that are taken for the six basic variables involved in Step 1 with the prescription that $[r_i, p_j] = ih\delta_{ij}$. On the contrary, within our scheme we recall that the six independent noncanonical variables A_i, L_i, ψ, $(\mathbf{AL}) = 0$ parametrize the phase space, i.e., any observable may be expressed as a function of them, and we suggest taking them as the basic variables and replacing them by six operators $\hat{A}_i$, $\hat{L}_i$, $\hat{\psi}(\hat{\mathbf{A}}\hat{\mathbf{L}} = 0)$, reproducing the algebraic relations (2.8)-(2.10), (2.22)-(2.24) in the sense of Step 1.

And what is more we find it useful to take for $\hat{A}_i$, $\hat{L}_i$ the exact generators of the $O(4)$ Lie algebra obeying the commutation relations

$$\begin{aligned} [\hat{L}_i, \hat{L}_j] &= ih\epsilon_{ijk}\hat{L}_k \\ [\hat{L}_i, \hat{A}_j] &= ih\epsilon_{ijk}\hat{A}_k \\ [\hat{A}_i, \hat{A}_j] &= ih\epsilon_{ijk}\hat{L}_k \end{aligned} \tag{3.1}$$

which coincide after being multiplied by ih, with the Poisson-bracket relations (2.8)-(2.10) *literally* and not only in the $h \to 0$ limit (thus exceeding the requirement stated in Step 1). As for the other basic variable ψ, we replace it by an operator $\hat{\psi}$, described in agreement with Step 1 as follows. It commutes with $\hat{L}_i$ [cf. (2.22)]

$$[\hat{\psi}, \hat{L}_i] = 0 \tag{3.2}$$

and with the operator $\hat{A}_i * 1/\hat{A}$ serving as the quantum analog of the observable A_i/A involved in (2.23) (the asterisk here denotes a special multiplication prescription to be specified below):

$$[\hat{\psi}, \hat{A}_i * (1/\hat{A})] = 0 \tag{3.3}$$

As for the last Poisson-bracket relation (2.24), it is reproduced in the $h \to 0$ limit by the commutator

$$\frac{1}{ih}[\hat{\psi}, (2\hat{G} + h^2)^{1/2}] = 1 \tag{3.4}$$

The algebraic reason why we take $(2\hat{G} + h^2)^{1/2}$ instead of $(2\hat{G})^{1/2}$ will become clear later when we see that the operator $(2\hat{G} + h^2)^{1/2}$ is the quantum analog for the Z_3 generator of the $O(2.1)$ algebra [see (5.9) and (5.10) below].

The commutation relations (3.1)-(3.4) define the six basic operators $\hat{A}_i$, $\hat{L}_i$, $\hat{\psi}$ of Step1. A matrix representation of these commutation relations will be described in Section 4.

To avoid a possible misunderstanding, it is worth emphasizing here that the consistency of the quantization under consideration is not influenced by whether the commutation relations (3.1)-(3.4) may be induced by the replacement $r_i \to \hat{r}_i$, $p_i \to \hat{p}_i$ (inherent in the canonical quantization) within the classical expressions of A_i, L_i, ψ in terms of r_i, p_i. One must realize that the operators $\hat{A}_i$, $\hat{L}_i$, $\hat{\psi}$ are taken as *primary* quantities representing the given algebra of commutation relations. This question and the role the answer to it may play within the present approach will be discussed in the concluding section, Section 6.

Now we pass to the discussion of the quantum definition of the energy (Step 2).

Within the usual canonical quantization scheme it is usual to postulate that the quantum Hamiltonian is merely the same function of the operators $\hat{\mathbf{r}}$, $\hat{\mathbf{p}}$ as the classical Hamiltonian was of $\mathbf{r}$, $\mathbf{p}$. This way of defining the quantum dynamics seems extremely natural[3] because the Hamiltonian (2.1) is a sum of the r- and p-dependent terms, and thus no question arises about the ordering of the noncommuting operators $\hat{\mathbf{r}}$, $\hat{\mathbf{p}}$. On the contrary, within the present quantization scheme we suggest (I) taking for the quantum Hamiltonian the same function $H(\hat{G}, \hat{L}^2)$ as the one obtained by reversing equation (2.6):

$$H(G, L^2) \to H(\hat{G}, \hat{L}^2) = \hat{H} \tag{3.5}$$

[3] This seems so natural that any other possibility is often overlooked altogether.

Again, since $[\hat{G}, \hat{L}^2] = 0$, no question arises of how to order the operators inside the function H. Since $\hat{G}$ and $\hat{L}^2$ are Hermitian and the classical energy is a real function, the Hamiltonian (3.5) is Hermitian. This is an illustration of the fact that the different sets of basic variables have led to different natural ways of defining the observable (energy), because it must be clear that the Hamiltonian (3.5) does differ from the Hamiltonian

$$\hat{H}_{\text{can}} = \tfrac{1}{2}\hat{p}^2 + V(\hat{r}) \tag{3.6}$$

of the canonical quantization. They coincide only in the $h \to 0$ limit. The fact that the use of different variables (even if they are connected by a canonical transformation) leads, generally, to different quantizations has been recognized as early as the very outset of the quantum mechanics (Tamm, 1926). It is easily seen [I] that the spectrum of the Hamiltonian (3.5) is to be obtained by the substitution of the eigenvalues of $\hat{G}$ and $\hat{L}^2$ $[\frac{1}{2}h^2(n^2 - 1), h^2 l(l + 1)$, respectively, where $l = 0, 1, 2, \ldots, n, n = 1, 2, 3 \ldots]$ into (2.6). This is apparently the Bohr-Sommerfeld rule, leading to what is usually referred to as the quasiclassical spectrum. It coincides with the spectrum of (3.6) only in the $h \to 0$ limit.

One may ask whether there exists a physical criterion to favor one choice of quantum dynamics over another. It is widely recognized that no such criterion exists (cf. e.g., Berezin, 1975). A possible objection that "the experimentally measured spectra and scattering amplitudes perfectly agree with their values calculated according to the canonical quantization scheme with the Hamiltonian (3.6)" is likely to relate only to the Coulomb case $V(r) = 1/r$. It is quite easy, however, to slightly modify our way of choosing the quantum Hamiltonian (3.5) so as to provide the exact coincidence of the resulting spectrum with that of (3.6) for the hydrogen atom. To meet this "hydrogen correspondence principle" it is sufficient to replace

$$2\hat{G} \to 2\hat{G} + h^2 \tag{3.7}$$

in (3.5), just as we did when passing from (2.24) to (3.4). This replacement creates the replacement $n^2 - 1 \to n^2$ in the spectrum. In the hydrogen atom case n is the same as the principle quantum number, and this replacement is enough to convert the quasiclassical spectrum into the exact spectrum of (3.6). We shall see below that the same replacement (3.7) appears as one out of a set of rules naturally arising within the present algebraic framework at Step 3 for defining other observables proceeding from their classical expressions.

4. *Matrix Representation for Basic Operators*

Now we proceed to develop the program of quantization sketched above.

For the generators $\hat{\mathbf{A}}$, $\hat{\mathbf{L}}$ of the $O(4)$ algebra obeying the relation $(\hat{\mathbf{L}}\hat{\mathbf{A}}) = 0$, which serves as a quantum generalization of equation (2.11), we take the

following matrix form (see, e.g., Gel'fand et al., 1958);

$$\langle n'l'm'|\hat{L}_3|nlm\rangle = hm\delta_{nn'}\delta_{ll'}\delta_{mm'}$$
$$\langle n'l'm'|\hat{L}_\pm = \hat{L}_1 \pm i\hat{L}_2|nlm\rangle = h\delta_{nn'}\delta_{ll'}\delta_{m',m\pm1}\,[(l \pm m + 1)(l \mp m)]^{1/2} \tag{4.1}$$

$$\langle n'l'm'|\hat{A}_3|nlm\rangle = ih\delta_{nn'}\delta_{mm'}\{\alpha(l, m)(n^2 - l^2)^{1/2}\delta_{l',l-1} - \alpha(l + 1, m)\delta_{l',l+1}\,[n^2 - (l + 1)^2]^{1/2}\}$$
$$\langle n'l'm'|\hat{A}_\pm|nlm\rangle = ih\delta_{nn'}\delta_{m',m\pm1}\{\pm\beta_1(l, \pm m)(n^2 - l^2)^{1/2}\delta_{l',l-1} \mp \beta_2(l, \pm m)\delta_{l',l+1}\,[n^2 - (l + 1)^2]^{1/2}\} \tag{4.2}$$
$$\hat{A}_\pm = \hat{A}_1 \pm i\hat{A}_2$$

which they have in the degenerate representation characterized by the special eigenvalue of the second Casimir operator $\hat{\mathbf{A}}\hat{\mathbf{L}} = 0$. In (4.2)

$$\alpha(l, m) = \left[\frac{(l - m)(l + m)}{4l^2 - 1}\right]^{1/2} \tag{4.3}$$

$$\beta_1(l, m) = \left[\frac{(l - m)(l - m - 1)}{4l^2 - 1}\right]^{1/2}$$

$$\beta_2(l, m) = -\left[\frac{(l + m + 1)(l + m + 2)}{4(l + 1)^2 - 1}\right]^{1/2}$$

The matrices (4.1), (4.2) obey the commutation relations (3.1). The basis $|n, l, m\rangle$ to which the matrices (4.1), (4.2) refer consists of vectors labeled by the integral numbers n, l, m, subject to the inequalities

$$-l \leqslant m \leqslant l, \qquad 0 \leqslant l < n, \qquad n = 1, 2, 3 \ldots \tag{4.4}$$

They are eigenvalues of the Casimir operators of the $SO(4)$ and its $SO(3)$ and $SO(2)$ subgroups:

$$\langle n'l'm'|2\hat{G}|nlm\rangle = (n^2 - 1)h^2\delta_{nn'}\delta_{ll'}\delta_{mm'} \tag{4.5}$$
$$\langle n'l'm'|\hat{L}^2|nlm\rangle = l(l + 1)h^2\delta_{nn'}\delta_{ll'}\delta_{mm'} \tag{4.6}$$
$$\langle n'l'm'|\hat{L}_3|nlm\rangle = mh\delta_{nn'}\delta_{ll'}\delta_{mm'} \tag{4.7}$$

Here $2\hat{G} = \hat{A}^2 + \hat{L}^2$. We may define the operator $\hat{\psi}$ in the same representation through its exponential

$$\hat{e}_\pm = \exp(\pm i\hat{\psi}) \tag{4.8}$$
$$\langle n', l', m'|\hat{e}_-|nlm\rangle = \delta_{n',n-1}\delta_{l'l}\delta_{m'm} \tag{4.9}$$
$$\langle n', l', m'|\hat{e}_+|nlm\rangle = \delta_{n',n+1}\delta_{l'l}\delta_{m'm} \tag{4.10}$$

From (4.9) and (4.10) it follows that the product e_+e_- is equal to unity, as it should be from (4.8): $e_+e_- = e^{-i\hat{\psi}}e^{i\hat{\psi}} = 1$. Also $[\hat{e}_+, \hat{e}_-] = 0$. Matrices (4.9) and (4.10) obviously commute with (4.1) and thus (3.2) is guaranteed. The commutation relation

$$[\hat{e}_\pm, (2\hat{G} + h^2)^{1/2}] = \mp h\hat{e}_\pm \tag{4.11}$$

follows from (4.9) and (4.10) and entails (3.4). Here

$$\langle n'l'm'|(2\hat{G} + h^2)^{1/2}|nlm\rangle = hn\delta_{nn'}\delta_{ll'}\delta_{mm'} \tag{4.12}$$

To achieve (3.3) with (4.8)-(4.10) it is necessary to define appropriately a quantum generalization of the unit vector $\mathbf{A}/A$. To this end note that the matrix of $\hat{A} = (2\hat{G} - L^2)^{1/2}$ is $h[n^2 - 1 - l(l+1)]^{1/2}\delta_{nn'}\delta_{ll'}\delta_{mm'}$. This square root differs from the n-containing square roots in (4.2) only by finite fixed additions to n^2 and l. For large quantum numbers $n, l \to \infty$ these additions are negligible, and thus in the quasiclassical limit the square roots coincide. Therefore expressions (4.2) with the n-containing square roots canceled out of them may play part of the quantum generalization of $\mathbf{A}/A$ denoted as $\hat{\mathbf{A}} * (\hat{A})^{-1}$:

$$\langle n'l'm'|\hat{A}_3 * \hat{A}^{-1}|nlm\rangle = i\delta_{nn'}\delta_{mm'}[\alpha(l, m)\delta_{l',l-1} - \alpha(l+1, m)\delta_{l',l+1}] \tag{4.13}$$

$$\langle n'l'm'|\hat{A}_\pm * \hat{A}^{-1}|nlm\rangle = i\delta_{nn'}\delta_{m',m\pm1}[\pm\beta_1(l, \pm m)\delta_{l',l-1} \mp \beta_2(l, \pm m)\delta_{l',l+1}]$$

These matrices obviously commute with (4.9)-(4.10), and (3.3) is thus satisfied.

Now the explicit construction of the operators $\hat{\mathbf{L}}$, $\hat{\mathbf{A}}$, $\hat{\psi}$ is completed. We do not dwell on Step 2 of quantization because it was described fully enough in our previous work (Serebrennikov and Shabad, 1973) and in the previous section. We proceed directly to Step 3.

5. *Quantum Definition of SO(4.2) Generators and Ordering Rules*

In this section we take the generators of $O(2.1)$, $O(4.1)$, and $O(4.2)$ as examples of quantum observables that may be defined in accordance with the correspondence principle using the matrix representations of the basic operators (4.1), (4.2), (4.8), and (4.9). In the H atom these noncompact groups were first considered by Barut (1964), Malkin and Man'ko (1965, 1966), Barut et al. (1966), and Böhm (1966).

Let us write first the generators of the algebras $SO(4.1)$, $SO(4.2)$, and $SO(2.1)$ operating in the phase space of the corresponding classical problem. The observables

$$\mathbf{B} = (2G)^{1/2}\left[\frac{\mathbf{A}}{A}\cos\psi - \frac{L}{(2G)^{1/2}}\sin\psi\,\frac{\mathbf{A}\times\mathbf{L}}{AL}\right] \tag{5.1}$$

$$B_4 = A\sin\psi \tag{5.2}$$

obey the following Poisson-bracket relations:

$$\begin{aligned}
\{L_i, B_j\} &= \epsilon_{ijk} B_k \\
\{A_i, B_j\} &= \delta_{ij} B_4 \\
\{L_i, B_4\} &= 0 \\
\{A_i, B_4\} &= -B_i \\
\{B_i, B_j\} &= -\epsilon_{ijk} L_k \\
\{B_4, B_i\} &= A_i
\end{aligned} \tag{5.3}$$

which form the $SO(4.1)$ algebra when combined with (2.8)-(2.10). The generators (5.1) and (5.2), for the Kepler case, coincide with those built by Bacry (1966) with the special value of his arbitrary parameters. The choice of the parameters made is dictated by the considerations (to be published elsewhere) analogous in spirit to those which have led to the unique determination of the precession vector (2.3). These considerations refer to a dynamical sense of the generators and to the requirement that they be members of the wider $SO(4.2)$ algebra. The latter is formed if the following four generators D_i, D_4 are added:

$$\mathbf{D} = -(2G)^{1/2} \left[\frac{\mathbf{A}}{A} \sin \psi + \frac{L}{(2G)^{1/2}} \cos \psi \, \frac{\mathbf{A} \times \mathbf{L}}{AL} \right] \tag{5.4}$$

$$D_4 = A \cos \psi \tag{5.5}$$

which obey the same bracket relations (5.3) as the B's do and commute with the latter in the following way:

$$\begin{aligned}
\{B_i, D_j\} &= \delta_{ij} D_5, \qquad \{B_4, D_4\} = D_5 \\
\{B_4, D_j\} &= \{B_j, D_4\} = 0
\end{aligned} \tag{5.6}$$

The observables (2.3), (2.5), (5.1), (5.2), (5.4), and (5.5) along with the observable

$$D_5 = (2G)^{1/2} \tag{5.7}$$

obeying the relations

$$\begin{aligned}
\{L_i, D_5\} &= \{A_i, D_5\} = 0 \\
\{D_4, D_5\} &= -B_4, \qquad \{B_4, D_5\} = D_4 \\
\{D_i, D_5\} &= -B_i, \qquad \{B_i, D_5\} = D_i
\end{aligned} \tag{5.8}$$

form the $SO(4.2)$ algebra of the Poisson brackets. The three observables B_4, D_4, and D_5 form the $SO(2.1)$ algebra among themselves:

$$\begin{aligned}
\{Z_3, Z_+\} &= -iZ_+ \\
\{Z_3, Z_-\} &= iZ_- \\
\{Z_+, Z_-\} &= iZ_3
\end{aligned} \tag{5.9}$$

where we have introduced the designations

$$Z_3 = D_5 = (2G)^{1/2}$$
$$Z_\pm = \frac{1}{\sqrt{2}}(B_4 \mp iD_4) = \mp\frac{i}{\sqrt{2}}(2G - L^2)^{1/2} e^{\pm i\psi} \tag{5.10}$$

Now we are in a position to give quantum definitions to the generators (5.1), (5.2), (5.4), (5.5), and (5.7). We start with the $O(2.1)$ algebra (5.9). Consider the operators $\hat{Z}_\pm$ given in the representation of the previous section by the matrices

$$\begin{aligned}\langle n'l'm'|\hat{Z}_+|nlm\rangle &= (-ih/\sqrt{2}[(n-l)(l+n+1)]^{1/2}\delta_{n',n+1}\delta_{ll'}\delta_{mm'}\\ \langle n'l'm'|\hat{Z}_-|nlm\rangle &= (ih/\sqrt{2}[(n+l)(n-l-1)]^{1/2}\delta_{n',n-1}\delta_{ll'}\delta_{mm'}\end{aligned} \tag{5.11}$$

which along with the operator $\hat{Z}_3 = [2\hat{G} + h^2]^{1/2}$ (4.12) provide the Lie algebra $O(2.1)$:

$$\begin{aligned}[\hat{Z}_3, \hat{Z}_\pm] &= \pm h\hat{Z}_\pm\\ [\hat{Z}_+, \hat{Z}_-] &= -h\hat{Z}_3\end{aligned} \tag{5.12}$$

Just as we did for $\hat{\mathbf{A}} * \hat{A}^{-1}$, we may easily make sure by substituting (4.9) and (4.10) into (5.10) that the latter coincides with (4.12) and (5.11) within quasi-classical accuracy. Therefore (4.12) and (5.11) may be regarded as appropriate quantum definition of the observables (5.10), which in the quantum case are generators of the $SO(2.1)$ group as equations (5.10) were in the classical case.

On the other hand we can abstract out from this example a rule which may be useful for defining other observables as well. To get (4.12) and (5.11) from (5.10) we must first apply to the latter the replacement (3.7). This immediately turns Z_3 into $\hat{Z}_3$ (4.12). After (3.7) is adopted and (4.9) and (4.10) are substituted into $Z_\pm$ (5.10) we prescribe a special law denoted by the double asterisks for the two factors in $Z_\pm$

$$\hat{Z}_\mp = \mp(i/\sqrt{2}) \overset{*}{*} (\hat{Z}_3{}^2 - L^2)^{1/2} e^{\pm i\hat{\psi}} \overset{*}{*} \tag{5.13}$$

The double-asterisk ordering is defined as follows (f is an arbitrary function of operators):

$$\langle n'l'm'| \overset{*}{*} f(\hat{Z}_3{}^2, e^{i\hat{\psi}}, e^{-i\hat{\psi}}) \overset{*}{*} |nlm\rangle = \langle n'l'm'| f(nn', e^{i\hat{\psi}}, e^{-i\hat{\psi}}|nlm\rangle \tag{5.14}$$

Its effect is to "average" the diagonal operator $\hat{Z}_3{}^2 = h^2 n^2 \delta_{nn'}\delta_{ll'}$ between the initial and final states. In accordance with the definition (5.14) the matrices of (5.13) coincide precisely with (5.11). For the more special case of the product $f(\hat{Z}_3{}^2)e^{\pm i\hat{\psi}}$ (which is the only case we will need) the double-asterisk ordering (5.14) reduces to the Weyl symmetrization,

$$W[f_1(\hat{Z}_3), f_2(\hat{\psi})] \equiv \int \tilde{f}_1(\alpha)\tilde{f}_2(\beta) e^{i(\alpha\hat{Z}_3 + \beta\hat{\psi})} d\alpha\, d\beta \tag{5.15}$$

[here $\tilde{f}_1(\alpha), \tilde{f}_2(\beta)$ are Fourier transforms of $f_1(\hat{Z}_3)$ and $f_2(\hat{\psi})$, respectively] after the extra replacement $\hat{Z}_3{}^2 \to \hat{Z}_3{}^2 - \frac{1}{4}h^2$ is made:

$$\begin{aligned}\hat{Z}_\pm &= \mp(i/\sqrt{2})\, W[(\hat{Z}_3{}^2 - \hat{L}^2 - \tfrac{1}{4}h^2)^{1/2} e^{\pm i\hat{\psi}}] \\ &= \mp(i/\sqrt{2})\, [(\hat{Z}_3 \mp \tfrac{1}{2}h)^2 - \hat{L}^2 - \tfrac{1}{2}h^2]^{1/2} e^{\pm i\hat{\psi}} \\ &= \mp(i/\sqrt{2}) e^{\pm i\hat{\psi}}\, [(\hat{Z}_3 \pm \tfrac{1}{2}h)^2 - \hat{L}^2 - \tfrac{1}{4}h^2]^{1/2}\end{aligned} \tag{5.16}$$

In deriving (5.16) the property (4.11) of $e^{\pm i\hat{\psi}}$ to be the shift operator was used. Equation (5.16) has the matrix form (5.11). Alternatively, one might obtain (5.16) by postulating the replacements (3.7) and $\hat{L}^2 \to \hat{L}^2 + \frac{1}{4}h^2$ and the Weyl symmetrization in $Z_\pm$ (5.10). Of course, the additional replacements $\hat{Z}_3{}^2 \to \hat{Z}_3{}^2 - \frac{1}{4}h^2$ or $\hat{L}^2 \to \hat{L}^2 + \frac{1}{4}h^2$ are not necessary as far as one wants to provide the commutation relations (5.12). With the $\frac{1}{4}h^2$ term omitted from (5.16), however, the Casimir invariant $Z_3{}^2 - Z_-Z_+ - Z_+Z_-$ of the $O(2.1)$ algebra would be equal to $\hat{L}^2 - \frac{1}{4}h^2$ and not to $\hat{L}^2$ as it is for (5.16) or (5.11).

Now that the quantum generators $\hat{Z}_\pm, \hat{Z}_3$ of the $SO(2.1)$ group are defined with their classical limit coinciding with the classical functions (5.10) of $\mathbf{A}$, $\mathbf{L}$, and ψ the definition of the generators of the $SO(4.2)$ may be given in the following way.[4] First we identify $\hat{Z}_\pm = (1/\sqrt{2})(\hat{B}_4 \mp i\hat{D}_4)$ (5.11), $D_5 = \hat{Z}_3 = (2\hat{G} + h^2)^{1/2}$ (4.12). The generators $\hat{\mathbf{D}}$ and $\hat{\mathbf{B}}$ are defined as the commutators: $\hat{\mathbf{D}} = [\hat{D}_4, \hat{\mathbf{A}}]\,(1/ih)$, $\hat{\mathbf{B}} = [\hat{B}_4, \hat{\mathbf{A}}]\,(1/ih)$. The corresponding matrices for $\hat{\mathbf{B}}$ and $\hat{\mathbf{D}}$ obtained by the commutations coincide with the standard matrices for the generators of the $O(4.2)$ algebra belonging to the continuous series of the unitary irreducible representation of this group (see, e.g., Böhm, 1966, for B's: put $\alpha = 0$ in Böhm's expressions)

$$\begin{aligned}\langle n'l'm'|\hat{B}_3|nlm\rangle = -\tfrac{1}{2}ih\delta_{m'm}\{&\delta_{l',l+1}\delta_{n',n+1}\alpha(l+1,m)[(n+l+1)(n+l+2)]^{1/2} \\ &- \delta_{l',l-1}\delta_{n',n+1}\alpha(l,m)[(n-l)(n-l+1)]^{1/2} \\ &+ \delta_{l',l+1}\delta_{n',n-1}\alpha(l+1,m)[(n-l-1)(n-l-2)]^{1/2} \\ &- \delta_{l',l-1}\delta_{n',n-1}\alpha(l,m)[(n+l)(n+l-1)]^{1/2}\}\end{aligned} \tag{5.17}$$

The matrix elements of $\hat{B}_\pm = [\hat{B}_4, \hat{A}_\pm]\,(1/ih)$ are obtained from (5.17) by the formal replacement, as in (4.2),

$$\delta_{mm'} \to \delta_{m',m\pm1} \qquad \alpha(l,m) \to \pm\beta_1(l,\pm m) \qquad \alpha(l+1,m) \to \pm\beta_2(l,\pm m) \tag{5.18}$$

where α and $\beta_{1,2}$ are given by (4.3).

$$\begin{aligned}\langle n'l'm'|\hat{D}_3|nlm\rangle = -\tfrac{1}{2}h\delta_{m'm}\{&-\delta_{l',l+1}\delta_{n',n+1}\alpha(l+1,m)[(n+l+1)(n+l+2)]^{1/2} \\ &+ \delta_{l',l-1}\delta_{n',n+1}\alpha(l,m)[(n-l)(n-l+1)]^{1/2} \\ &+ \delta_{l',l+1}\delta_{n',n-1}\alpha(l+1,m)[(n-l-1)(n-l-2)]^{1/2} \\ &- \delta_{l',l-1}\delta_{n',n-1}\alpha(l,m)[(n+l)(n+l-1)]^{1/2}\}\end{aligned} \tag{5.19}$$

[4] For the Coulomb case this group was discovered by Malkin and Man'ko (1965, 1966).

The matrix elements of $\hat{D}_\pm = [\hat{D}_4, \hat{A}_\pm](1/ih)$ are obtained from this again by the formal substitution (5.18).

The coincidence, in the $h \to 0$ limit, of these matrices for $\hat{D}_3$, $\hat{D}_\pm$, $\hat{B}_3$, and $\hat{B}_\pm$ with those that may be obtained from D_3, $D_\pm$, B_3, and $B_\pm$, (5.4), (5.1) by substitution of (4.1), (4.2), (4.9), and (4.10) is provided by the fact that in this limit every commutator between two operators, say $\hat{X}$ and $\hat{Y}$, divided over ih should coincide with the result of the Poisson-bracket calculation $\{X, Y\}$ once the classical quantities X, Y are classical limits of $\hat{X}$ and $\hat{Y}$, respectively. This property of the quantum multiplication law necessarily imposed on the basic operators $\hat{A}_i$, $\hat{L}_i$, $\hat{\psi}$ (see Section 3) was seen in Section 4 to be fulfilled for their matrix representation considered. Thus it also holds for all the other observables (including $\hat{B}_4$, $\hat{D}_4$) that are functions of them. The coincidence in the classical ($n \gg 1$) limit of $\hat{\mathbf{B}}, \hat{\mathbf{D}}$ with their classical expressions may be also verified directly.

6. *Concluding Remarks*

To judge at which step the quantization here described becomes non-equivalent with the canonical one, it is important to answer the question of whether the substitution of the operators, subject to the commutation relations (3.1)–(3.4), for the basic observables $\mathbf{A}$, $\mathbf{L}$, and ψ may be induced by the canonical procedure of replacing $\mathbf{r}$ and $\mathbf{p}$ by the operators obeying the relation $[\hat{r}_i, \hat{p}_j] = ih\delta_{ij}$ inside the classical functions (2.5), (2.3), and (2.21). This possibility is obvious for the angular momentum subalgebra in (3.1) produced directly by the expression $\hat{L}_i = \epsilon_{ijk}\hat{r}_j\hat{p}_k$. For the Coulomb case the Weyl symmetrization between $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ within the expression of the Runge–Lenz vector is known to lead to (3.1). In the general case no such procedure is known. At present we are able to prove the following statement, which relates to the harmonic oscillator (to be published elsewhere): Take the eigenstates of the Hamiltonian (3.6) with $V(r) = \omega^2 r^2$ as the vectors $|n, l, m\rangle$ of Sections 4 and 5 with l and m recognized as the orbital and magnetic quantum numbers, respectively, and n as the sum $n = n_r + l + 1$, where n_r is the radial quantum number. Then calculate the matrix elements of the canonical variables $\langle n'l'm'|\hat{\mathbf{r}}, \hat{\mathbf{p}}|n, l, m\rangle$ and substitute the result into (2.3). The resulting matrix expressions coincide within the accuracy of h with the matrices (4.2). This implies that in this particular case quantum generators of the $SO(4)$ algebra do exist that differ from the arbitrarily ordered corresponding classical functions of the operators of canonical position and momentum no more than within the accuracy of h. We believe that this result must hold for the general potential as well. We must emphasize once again, however, that no matter how the question under discussion is answered, the validity of the construction of the body of the paper is not affected.

Note added in proof. The question asked in Section 6 may be answered in the positive for the general potential.

Proof: In the $h \to 0$ limit quantum operators turn into classical expressions whose Poisson bracket relations are the same as the commutation relations

of their operator prototypes. This applies to the quantum generators of $SO(4)$, defined as operators whose matrix elements with respect to the eigenstates of the canonical Hamiltonian (3.6), labeled as in Section 6, are given by (4.1), (4.2). Expressions (2.3), (2.4), (2.7), with (2.6) yet unknown, are the most general expressions satisfying (2.5) and the Poisson bracket relations of the $SO(4)$ algebra shown in I. The basic vectors $|n, l, m\rangle$ correspond to the energy eigenvalues $H(n, l) = H(n_r + l + 1, l)$.

By going to the Bohr–Sommerfeld limit of this expression and expressing n in terms of G with the help of (4.12), one obtains (2.6). Thus our precession vector [(2.3), (2.4), and (2.6)] is the classical limit of the quantum $SO(4)$ generators created within the canonical quantization scheme. The analogous statement holds for ψ. Therefore the present quantization differs from the canonical one only as far as Steps 2 and 3 are concerned. Details of the limiting transition will be traced in a separate publication.

Acknowledgments

We wish to thank Professors F. A. Berezin, E. S. Fradkin, and Ya. A. Smorodinsky for helpful discussions and advice.

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