On the Group Quantization of Constrained Systems

— A Simple Non-Trivial Model —

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The group quantization method is one of the promising methods for quantization of systems with 1st class constraints such as the general theory of relativity. For the investigation of the structure of group quantization, we present a simple model—the 2-dimensional Kepler model—which has sufficiently rich physical contents. Even for this simple model, the group quantization reveals its various properties. Above all, it is explicitly shown that the group quantization method cannot automatically solve the operator ordering problem. We compare the group quantization and the Dirac method with each other in reference to our model. The extension of our model to more general cases is also discussed.

§ 1. Introduction

The general theory of relativity can be regarded as a dynamical system with four 1st class constraints, which are connected with the covariance of the theory under coordinate transformations.\(^1\) For the quantization of 1st class constrained systems, such as the relativity theory, there is another prescription called the group quantization method,\(^2\),\(^3\) besides the well-known Dirac method.\(^4\)

The group quantization method has not yet been so deeply pursued, in spite of its uniqueness and potentiality. One reason for this situation may be its difficulty and complexity in practical execution, especially the difficulty in finding out the symmetry group \(G\) of the phase space, which plays an essential role in group quantization. As a result, there are few practical examples, some of which are quite physically trivial and others of which are too special and complicated,\(^2\),\(^3\),\(^5\) to see the essential feature of the method with clear physical intuition.

The purpose of this paper is to provide a model, which is sufficiently simple for execution of group quantization and which has at the same time adequately rich physical contents. We hope that it will serve as a preliminary toy-model for the investigation of the group quantization of constrained systems, just like a harmonic oscillator for the usual quantum mechanics.

In some literature,\(^3\) it is asserted that one can skip the explicit operator ordering fixation in the group quantization, because the symmetry group \(G\), which is purely a classical object, plays a central role in this method. We mainly concentrate on this point in this paper with our simple model: Whether or not the above assertion is true.

After reviewing essential points of the group quantization method in the next section, we provide our model, the 2 dimensional Kepler model, in § 3 and study it on the lines of group quantization. We find out explicitly that the precise ordering fixation is indispensable for obtaining physical information and that the group quantization is not more advanced than the Dirac method on this point. Keeping this...
observation in mind, we consider more about the operator ordering problem in § 4, and give some speculations about how uniquely the group quantization method fixes the orderings. In § 5, we study the same model on the lines of the Dirac method for comparison's sake. Regarding the results of the group quantization in § 3 as a guidance, we here obtain some insights into the ordering fixation problem in the Dirac method. In § 6, we sketch how to extend our model to a general Lie group. It is discussed that the key tool for construction is the Casimir operators. Section 7 is devoted to the comparison with both methods, the group quantization and the Dirac method, and we point out some difficulties proper to each method.

§ 2. Group quantization

When the classical phase space \( S \) of some system is given, one usually quantizes the system by the following procedure:

1. \( \{q, p\}_{PB}=1 \rightarrow [\hat{q}, \hat{p}]=i\hbar. \)
2. Construct a vector space \( \mathcal{H} \) with some inner product \( (, ) \) s.t. \( \hat{q} \) and \( \hat{p} \) become Hermitean operators on it.

In some cases, however, one does not rely on the above procedure and goes on more directly. For example, when one part of the total degrees of freedom obeys the \( SU(2) \) Poisson-bracket algebra (angular momenta etc.), one quantizes the part as

\[ \{L_i, L_j\}_{PB} = \epsilon_{ijk} L_k \rightarrow \text{construct the unitary representation of } SU(2). \]

Extending this idea, one arrives at the group quantization. In group quantization, one regards the quantization procedure as

Quantization = Construction of the unitary representation of the (sufficiently big) Lie group \( G \), the canonical-transformation group on the phase space \( S \).

More precisely, the procedure consists of the following three steps:

(G1) Find out the Lie group \( G \) s.t. it acts on \( S \) transitively and effectively.
(G2) Find out physical quantities corresponding to generators of \( \mathcal{L}(G) = \text{Lie algebra of } G \).
(G3) Construct the irreducible unitary representation of \( G \).

There are some comments on these steps.

(G1): The physical meaning of "\( G \) acts on \( S \) transitively (i.e. \( \forall s, \forall s' \in S, \exists g \in G \) s.t. \( s'=g(s) \)"") is that all states (phase points) of the system are connected with each other by canonical transformations corresponding to \( G \). In other words, it means that one selects out a sufficient number of observables for quantization (because in (G2), one maps generators \( \{A_i, \ldots, A_n\} \) of \( \mathcal{L}(G) \) to observables \( \{f_1, \ldots, f_n\} \) for quantization). The meaning of "\( G \) acts on \( S \) effectively (i.e., \( \exists g \in G, \forall s \in S, g(s)=s \Rightarrow g = e \) (unit element))" is that one quantizes minimal observables (if \( G \) is not effective,
one can always obtain $G'$: effective, by $G' = G/K$ where $K := \{g \in G | g(s) = s$ for $\forall s \in S\}$ is the normal subgroup of $G$.

(G2): For $A \in \mathcal{L}(G)$, a vector field $\gamma^A$ on $S$ is defined by the $G$-action on $S$. (For a given $A$, draw a curve $c$ through $e$ in $G$ by the exp-map $\exp(-tA)$. Then draw a curve $\tilde{c}$ through $s(\in S)$ in $S$ by acting $c$ to $s$. Thus one gets $\gamma^A$, a tangent vector of $\tilde{c}$ at $s$.) If one finds out $f^A \in C^\infty(S, \mathbb{R})$ s.t. $\gamma^A(F) = [f^A, F]_{PB}$ for $\forall F \in C^\infty(S, \mathbb{R})$, for all generators $A's \in \mathcal{L}'(G)$, they follow $\{f_A, f_B\}_{PB} = [j_A, j_B]_{PB}$ (by a suitable redefinition $f^A \to f^A + c(\text{const})$). (Whether or not the $f^A$'s exist depends on the cohomology property of $\mathcal{L}(G)$; $H^2(\mathcal{L}(G); \mathbb{R}) = 0$ turns out to be a sufficient condition for the existence of the $f^A$'s. 

(G3): Let $U: G \to \mathcal{H}$ be a unitary representation of $G$ on a representation space $\mathcal{H}$ (therefore, generator $A \in \mathcal{L}(G)$ are represented as Hermitean operators on $\mathcal{H}$). By the way, in (G2), we have mapped $A's \in \mathcal{L}(G)$ to $f^A's \in C^\infty(S, \mathbb{R})$. Thus, we have automatically obtained a map $f^A's \in C^\infty(S, \mathbb{R}) \to \tilde{f}^A's$: Hermitean on $\mathcal{H}$. Moreover,

$$\begin{pmatrix}
\frac{1}{i} \tilde{f}^A, \\
\frac{1}{i} \tilde{f}^B
\end{pmatrix} = \frac{1}{i} [\tilde{j}^A, \tilde{j}^B]_{PB} \quad \text{by the construction of representation,}
\{f^A, f^B\}_{PB} = [j^A, j^B]_{PB} \quad \text{by (G2)}. $$

Thus, the Poisson-bracket algebra has been translated into the commutator algebra by the medium of the Lie-bracket algebra: $[f^A, f^B]_{PB} \to (1/i)[\tilde{j}^A, \tilde{j}^B]_{PB}$.

The last subject of this section is on a slight modification for the case when the system is subject to 1st class constraints $C_i(q, p) = 0$. In this case, the constraint surface $\Sigma := \{(q, p) \in S | C_i(q, p) = 0\}$ consists of orbits generated by the $C_i$'s, and the physical objects are $C_i$-orbits. Thus the physical phase space is $S_{\text{phys}} := \Sigma/C_i = \{C_i\text{-orbit}\}$. Thus, one has only to replace $S$ by $S_{\text{phys}}$ in the above procedure (G1-3). The step (G1) is especially replaced by the following (CG1-a) and (CG1-b):

(CG1-a) Find out a group $G$: $S_{\text{phys}} \to S_{\text{phys}}$, i.e., one $C_i$-orbit $\to$ one $C_i$-orbit. This statement can be expressed as $[f^A, C_i]_{PB} \approx 0$, where $f^A's \in C^\infty(S, \mathbb{R})$ are determined by $A's \in \mathcal{L}(G)$ in (G2).

(CG1-b) $G$ acts on $S_{\text{phys}}$ transitively and effectively.

A function $Q \in C^\infty(S, \mathbb{R})$ s.t. $\{Q, C_i\}_{PB} \approx 0$ is called a physical observable (or a Dirac observable). (CG1-a) says that function $f^A's \in C^\infty(S, \mathbb{R})$ corresponding to $A's \in \mathcal{L}(G)$ (step (G2)) are physical observables. Thus, a convenient way to find out $G$ is to find out independent physical observables and to study their Poisson-bracket algebra. In the next section, we proceed on these lines for a simple toy-model.

The most prominent advantage of the group quantization method is that one obtains physical states and the inner product on them automatically, once $G$ is found out and its representation is constructed. One need not solve the constraint equations nor to look for the appropriate inner product.

Once $G$ is found, one can perform the group quantization straightforwardly. The group $G$ itself is a classical object, which is some transformation group on the phase space $S$ (or $S_{\text{phys}}$).
One might consider that the group quantization method would provide us with the quantum theory directly from $G$ without suffering from complicated operator ordering problems. However, this expectation turns out to be false as we will see in the next section. What the group quantization method provides us is only the algebraic structure of the phase space and some other physically significant information requires extra considerations. Thus, one cannot skip the ordering fixation, which is often quite a hard task even for a simple model just like the usual Dirac method.

§ 3. The Kepler model

Let us examine the method of group quantization by applying it to a simple, non-trivial model, the Kepler model.

A point particle (mass $m$) moving in a centrifugal potential, $V(r)$, has a conserved angular momentum $L$. Furthermore, when the potential is a Kepler type, i.e., $V(r) = -(k/r)$ ($k$ in some constant), there is another conserved quantity, the so-called Laplace-Runge-Lenz vector (or an eccentricity vector)

$$A := p \times L - mk \frac{r}{\gamma}. \quad (1)$$

There are seven conserved quantities $E, L, A$, five of which are independent because of two identities,

$$\begin{align*}
A \cdot L &= 0, \quad (2a) \\
A^2 &= m^2 k^2 + 2mEL^2. \quad (2b)
\end{align*}$$

It is also known that $L$ and $D := (1/\sqrt{2mE})A$ work as the generators of some Lie algebra:

1. When $E < 0$, so$(4)$.
2. When $E > 0$, so$(3, 1)$.

$$\begin{align*}
\{L_i, L_j\}_P &= \epsilon_{ijk}L_k, \\
\{D_i, L_j\}_P &= \epsilon_{ijk}D_k, \\
\{D_i, D_j\}_P &= \pm \epsilon_{ijk}L_k
\end{align*}$$

and $D^2 \pm L^2 = \frac{mk^2}{2|E|}$ (for 1., $-$ for 2.).

3. When $E = 0$, $L$ and $A$ are the generators of algebra corresponding to $R^3 \otimes SO(3)$.

The above special group theoretical property of the Kepler system has a long history and its quantum mechanical significance was first recognized and investigated by Pauli.

As is well-known in classical mechanics, the motion of a particle in a centrifugal potential $V(r)$ is restricted to a plane, and hence we usually reduce the problem to a
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2-dimensional problem. In connection with this fact, corresponding formulas in quantum theory are expected to become much simpler in 2 dimensions than in full 3 dimensions. We thus study 2-dimensional Kepler model below. (We should note one point here: In quantum theory, the 2-dimensional Kepler model is a completely different system from the 3-dimensional counterpart, because the way that wave functions distribute entirely depends on the dimensionality.)

Moreover, we dare choose the polar coordinates \((r, \theta)\) (and \(\phi = (\pi/2)\)) with the aim of investigating the operator ordering problem in group quantization, because, in general, in the polar coordinates the ordering problem appears explicitly. Another motivation for introducing the polar coordinates is related with the quantum cosmology. If one regards \(r\) analogous to the scale factor \(a\), one obtains simple cosmology-oriented model suitable for the group quantization framework. Moreover, since \(r\) varies classically from \((1-\epsilon)R\) to \((1+\epsilon)R\) when \(E<0\), and from \((\epsilon-1)R\) to infinity when \(E>0\), this model is appropriate for the investigation of time problem in the Hamiltonian vanishing constrained systems \(^8\) (where \(R^2 = (k/2|E|, \epsilon = (1+2EL^2/mk^2)^{1/2})\).

Now, there remains the symmetry group even in the 2-dimensional Kepler system. Introducing the quantities

\[
\begin{align*}
  u_1 &= \frac{1}{\sqrt{2m|E|}} A_x = \frac{1}{\sqrt{2m|E|}} \left( \frac{1}{r} p_\theta^2 \cos \theta - mk \cos \theta + p_r p_\theta \sin \theta \right), \\
  u_2 &= \frac{1}{\sqrt{2m|E|}} A_y = \frac{1}{\sqrt{2m|E|}} \left( \frac{1}{r} p_\theta^2 \sin \theta - mk \sin \theta - p_r p_\theta \cos \theta \right), \\
  u_3 &= p_\theta, \\
  C &= \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} - \frac{k}{r} E.
\end{align*}
\]

we get

1. When \(E<0\), \(so(3)\), \(\{u_1, u_2\}_\text{PB} = \epsilon_{ijk} u_k\),

   \[u_1^2 + u_2^2 + u_3^2 = \frac{mk^2}{2|E|} + \frac{1}{|E|} u_3^2 C.\] (3-a)

2. When \(E>0\), \(so(2,1)\), \(\{u_1, u_2\}_\text{PB} = - u_3\)

   \[\{u_2, u_3\}_\text{PB} = u_1, \{u_3, u_1\}_\text{PB} = u_2\],

   \[u_1^2 + u_2^2 - u_3^2 = \frac{mk^2}{2E} + \frac{1}{E} u_3^2 C.\] (4-a)

3. When \(E=0\), \(A_x, A_y\) and \(p_\theta\) are the generators of algebra

   corresponding to \(R^2 \otimes U(1)\).

Now, consider the constrained system (corresponding to the 2-dimensional Kepler system) \(((r, p_r), (\theta, p_\theta); C \approx 0)\).

The physical observables (or Dirac observables) of this system are the \(u_i\)'s. (In the following, we mainly consider Case 1, \(E<0\). The same discussion can be made also for Case 2, \(E>0\).)
Noting that the $u_i$'s are physical observables, i.e., invariant under the action of $C$ \((u_i, C)_{PB}=0\), Eq. (4·b) (or (4'·b)) means that the physical phase space $S_{\text{phys}}$ can be neatly expressed by the system of coordinates $(u_1, u_2, u_3)$, three functions of $S$ (Eqs. (3·a~c)). Indeed, when $E<0$, $S_{\text{phys}}$ is expressed as a 2-sphere of radius $(mk^2/2|E|)^{1/2}$, whose center is at the origin of $(u_1u_2u_3)$-space (when $E>0$, $S_{\text{phys}}$ is described as a 2-hyperboloid). Note also that $(u_1, u_2, u_3)$ are physical observables, i.e., invariant under the action of $C$ \((u_i, C)_{PB}=0\). Eq. (4·b) (or (4'·b)) can be interpreted as the $SO(3)$- (or $SO(2, 1)$-) action of the $u_i$'s on the $(u_1, u_2, u_3)$-space. Thus, it is obvious that this action on the 2-sphere (or 2-hyperboloid) is transitive and effective, so that the conditions (CG1-a, b) mentioned in the previous section are satisfied.

We should also note that the mapping from \((r, p_r), (\theta, p_\theta)\) to $(u_1, u_2, u_3)$ is periodic in $\theta$ with the period $2\pi$ \(\theta\) only appears in Eqs. (3·a, b) by the form of $\sin \theta$ or $\cos \theta$). This periodicity is very natural, of course, because the original meaning of $\theta$ was the angle in the polar-coordinates, which we have chosen to describe the Kepler system. However, if we look upon the system $(r, p_r), (\theta, p_\theta); C\approx 0)$ as it is, discarding intentionally its original meaning, we are led to the more profound interpretation of the periodicity in $\theta$: The investigation of the group theoretical structure of $S_{\text{phys}}$ informs us of the periodicity of physical states in a certain variable, to know which is almost impossible from any other considerations. We will return on this point at the end of § 5.

Looking for the operators satisfying the above algebra, i.e.,

\[
\begin{bmatrix}
\tilde{u}_i, \tilde{u}_j \equiv i\hbar \epsilon_{ijk} \tilde{u}_k \\
[\tilde{u}_i, \tilde{C}] = 0
\end{bmatrix} \pmod{C},
\]

we obtain

\[
\begin{align*}
\tilde{u}_1 &:= \frac{1}{\sqrt{2m|E|}} \left\{ \frac{1}{\bar{r}} \langle \bar{p}_\theta \langle \bar{p}_\theta \cos \bar{\theta} \rangle \rangle - mk \cos \bar{\theta} + \bar{r}, \langle \bar{p}_\theta \sin \bar{\theta} \rangle \right\}, \\
\tilde{u}_2 &:= \frac{1}{\sqrt{2m|E|}} \left\{ \frac{1}{\bar{r}} \langle \bar{p}_\theta \langle \bar{p}_\theta \sin \bar{\theta} \rangle \rangle - mk \sin \bar{\theta} - \bar{r}, \langle \bar{p}_\theta \cos \bar{\theta} \rangle \right\}, \\
\tilde{u}_3 &:= \bar{p}_\theta, \\
\tilde{C} &:= \frac{\bar{p}_r^2}{2m} + \frac{\bar{p}_\theta^2 - \frac{1}{4} \hbar^2}{2m \bar{r}^2} - \frac{k}{\bar{r}} - E,
\end{align*}
\]

where $\langle AB \rangle := (1/2)(AB + BA)$.

The correct algebras (5·a, b) are recovered only by the above special ordering choice. In particular, we should note that the term $-(1/4)\hbar^2$ in (6·d) does not appear in the corresponding classical expression (or, one can say that $-(1/4)\hbar^2$ vanishes when $\hbar \to 0$). If this term had been omitted, one would not have obtained the correct algebras (5·a, b), and moreover, one would not have obtained the correct spectrum for $E$, as will be discussed below.

One example of the wrong orderings is shown for comparison's sake:
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Although these quantities satisfy (5·a) (mod \( \hat{C} \)), they do not satisfy (5·b), so that they are inappropriate as a result.

Now, by the above correct ordering (6·a ~ d), one gets as the quantum analogue of Eq. (4·b),

\[
\hat{u}_1^2 + \hat{u}_2^2 + \hat{u}_3^2 = \frac{mk^2}{2|E|} - \frac{1}{4} \hbar^2 + \frac{1}{|E|} \left( \hat{u}_3^2 + \frac{1}{4} \hbar^2 \right) \hat{C}.
\]  

(7)

On the other hand, as is well known in the representation theory of Lie algebra, the eigenvalues of \( \hat{u}_1^2 + \hat{u}_2^2 + \hat{u}_3^2 \) are restricted as

\[
\begin{pmatrix}
J=0 & 1 & 2 & 3 & \ldots \\
J=1/2 & 3/2 & 5/2 & \ldots
\end{pmatrix}
\]  

(8)

on a positive definite Hilbert space. Comparing (7) and (8) with each other, we conclude that only when the parameter \( E \) satisfies

\[
E_J = \frac{mk^2}{2\hbar} \frac{1}{(J+1/2)^2}
\]  

\[
\begin{pmatrix}
J=0 & 1 & 2 & 3 & \ldots \\
J=1/2 & 3/2 & 5/2 & \ldots
\end{pmatrix}
\]  

(9)

the unitary representation for \( SO(3) \), which is the symmetry group of the system in question, can be constructed.

Equation (7) relates generators with physical parameters, while Eq. (8) is a purely algebraic relation. We have obtained the energy spectrum (9) only after considering (7) and (8) simultaneously, i.e., only after translating an algebraic relation into a physical language. The formula which group quantization gives us (i.e., the \textit{classical} algebraic structure of the system tells us) is Eq. (8), while Eq. (7) can be obtained only after giving the explicit \textit{quantum} formulas (6·a ~ d), which define generators in terms of dynamical variables and fix the operator orderings. The physically significant relation (9) is therefore beyond the framework of group quantization, in a sense that \textit{one can never obtain} (9) \textit{only from the knowledge of the classical} \( SO(3) \text{ structure on the phase space of the system} \) (Eqs. (5·a, b)). In other words, the task for finding out the correct operator ordering, which is often a very hard task even for a simple system such as the Kepler model, cannot be skipped also in the group quantization approach just like the usual Dirac prescription.

Next, let us construct physical states. Using the simultaneous eigenstates of \( \hat{u}_1^2 \) and \( \hat{u}_3 \), \( |JM\rangle \), the states are constructed as
where the $c^M$'s are some coefficients. For fixed $J$, the state $|J\rangle$ can be interpreted as the superposition of elliptical orbits whose semimajor axes are of the common length $a = k/2|E_j| = \hbar^2(J + 1/2)^2/mk$.

Noting Eq. (7), it is obvious that the state $|J\rangle$ satisfies the "Wheeler-DeWitt equation",

$$\hat{C}|J\rangle = 0.$$  

We have thus constructed the physical state $|J\rangle$'s and defined unique inner product on them through the unitary representation of the symmetry group $SO(3)$, without solving the constraint equation (11). This point is the most prominent property of the group quantization method.

§ 4. The operator-ordering ambiguity

Let us consider more about the operator ordering problem.

The term "ordering problem", in a broad sense, implies the following two mutually independent contents:

(a) Technical difficulties for constructing the explicit well-ordered expressions of quantum operators from the classical counterparts.

(b) Uniqueness of these orderings.

Regarding (a), we have learned enough through our model how hard and tedious it is to find out the expressions like $(4\cdot a \sim b)$ (though we have totally omitted the description of the details for obtaining them). More significantly, we have learned that the well-ordered expressions like $(4\cdot a \sim d)$, which require patient manipulations, are indispensable for obtaining information such as Eq. (9), as opposed to the naive expectation stated at the last paragraph of § 2.

With respect to (b), it appears that the relations characterizing the Lie algebra such as $(5\cdot a, b)$ fix the orderings quite uniquely, though the rigorous proof for the uniqueness cannot be given here. Indeed, the relations $(5\cdot a, b)$ are tightly combined with each other so that even a slight change of orderings destroys them; We gave one example just before Eq. (7).

Let us try to formulate this uniqueness problem more generally. Consider that one has found out the well-ordered expressions for the $u_A$ which satisfy

$$[u_A, u_B] = i \hat{C}_{AB}^C u_C ,$$

(Equality in this section, including Eq. (12), should be regarded as mod $C$, if necessary.)

Let other expression $u_A$'s
also satisfy (12). Then the \( f_A \)'s should satisfy

\[
[u_A, f_B] + [f_A, u_B] - i \tilde{C}_{AB} \epsilon C = -[f_A, f_B].
\]

(13)

The shift \( f_A \), the candidate of the ordering ambiguity, should be of the form

\[
f_A = \frac{\hbar}{\sigma} f_A^{(1)} + \left( \frac{\hbar}{\sigma} \right)^2 f_A^{(2)} + \left( \frac{\hbar}{\sigma} \right)^3 f_A^{(3)} + \cdots
\]

(14)

where \( \sigma \) is any fixed constant such that \( [\sigma] = [\hbar] \).

Substituting (14) into Eq. (13) and extracting each equation for each order in \( \hbar \), one obtains (noting that \([\cdot, \cdot] \) and \( \tilde{C}_{AB} \epsilon C \) are of order \( \hbar \))

\[
[u_A, f_B^{(1)}] + [f_A^{(1)}, u_B] - i \tilde{C}_{AB} \epsilon C^{(1)} = 0,
\]

\[
[u_A, f_B^{(2)}] + [f_A^{(2)}, u_B] - i \tilde{C}_{AB} \epsilon C^{(2)} = -[f_A^{(1)}, f_B^{(1)}],
\]

\[
[u_A, f_B^{(3)}] + [f_A^{(3)}, u_B] - i \tilde{C}_{AB} \epsilon C^{(3)} = -[f_A^{(1)}, f_B^{(2)}] - [f_A^{(2)}, f_B^{(1)}],
\]

\[
\vdots
\]

thus

\[
[u_A, f_B^{(n)}] + [f_A^{(n)}, u_B] - i \tilde{C}_{AB} \epsilon C^{(n)} = -\sum_{k=1}^{n-1} [f_A^{(n-k)}, f_B^{(k)}]. \quad (n=1, 2, \ldots)
\]

(15)

If there exists a set of non-vanishing solution \( f_A^{(n)} \)'s for Eq. (15), there is a possibility of ordering ambiguity.

The necessary condition for \( f_A^{(n)} = F_A^{(n)}(\bar{q}, \bar{p}) \) to be a set of solutions for Eq. (15) is that \( \{F_A^{(n)}(q, p)\} \in C^\infty(S, R) \) satisfy the "classical analogue" of Eq. (15),

\[
[u_A, F_B^{(n)}]_{PB} + [F_A^{(n)}, u_B]_{PB} - \tilde{C}_{AB} \epsilon C^{(n)} = -\sum_{k=1}^{n-1} [F_A^{(n-k)}, F_B^{(k)}]_{PB}.
\]

(15')

\((n=1, 2, \ldots; A, B = 1, 2, \ldots, N = \dim G)\)

For each \( n \), there are \( nC_2 \) partial differential equations of 1st order, while there are \( N \) unknown functions. Thus Eq. (15) defines, as over-determined system for \( N > 3 \), so that there are not general solutions and there are at most special solutions, if any. This suggests that the relation (12) restricts the variety of allowed ordering very strongly, if not uniquely. Thus the group quantization method, in which one makes full use of Eq. (12), can be said to provide us a decisive resolution of the ordering problem in the sense of (b) in principle, although it is in the same position as the Dirac method with regard to (a).

For \( G = SU(2) \) (this is the \( N = 3 \) case), (15) becomes

\[
[u_A, f_B^{(1)}] + [f_A^{(1)}, u_B] = i\hbar f_A^{(1)}, \quad \text{(perm)}
\]

\[
[u_A, f_B^{(2)}] + [f_A^{(2)}, u_B] = i\hbar f_A^{(2)} - [f_A^{(1)}, f_B^{(1)}], \quad \text{(perm)}
\]

\[
[u_A, f_B^{(3)}] + [f_A^{(3)}, u_B] = i\hbar f_A^{(3)} - [f_A^{(1)}, f_B^{(2)}] - [f_A^{(2)}, f_A^{(1)}], \quad \text{(perm)}
\]

\[
\vdots
\]
where \((\text{perm})\) means the equation obtained from the just previous equation by the permutation of the lower indices, \(1 \rightarrow 2 \rightarrow 3 \rightarrow 1\).

There is a set of solutions

\[
\begin{align*}
\begin{cases}
  f_1^{(1)} = -u_2 \\
  f_2^{(1)} = u_1 \\
  f_3^{(1)} = 0
\end{cases}, & \begin{cases}
  f_1^{(2)} = -u_1/2! \\
  f_2^{(2)} = -u_2/2! \\
  f_3^{(2)} = 0
\end{cases}, & \begin{cases}
  f_1^{(3)} = -u_2/3! \\
  f_2^{(3)} = -u_1/3! \\
  f_3^{(3)} = 0
\end{cases}, & \ldots.
\end{align*}
\]

This is a trivial set of solutions because it comes from the freedom of generator-choice which already existed in the classical level: the \(u_i\)'s such that

\[
\begin{pmatrix}
  u_1' \\
  u_2'
\end{pmatrix} =
\begin{pmatrix}
  \cos \alpha & -\sin \alpha \\
  \sin \alpha & \cos \alpha
\end{pmatrix}
\begin{pmatrix}
  u_1 \\
  u_2
\end{pmatrix} \quad (\alpha \in \mathbb{R}),
\]

also satisfy (5·a). The above set of solutions can be regarded as a special case when \(\alpha = \hbar/\sigma\), thus it has nothing to do with the ordering ambiguity. One can speculate that there is no other set of solutions from the experience of finding out Eqs. (6·a~d) though it is difficult to give a proof of it.

§ 5. **The Dirac-Wheeler-DeWitt approach**

In this section, let us apply another method, the Dirac-Wheeler-DeWitt method, to the same model with the aim of comparison with the group quantization method discussed in the previous section.

The classical "Hamiltonian constraint" for the present model is

\[
C = p_r^2/2m + p^2/2mr^2 - k/r - E \approx 0.
\]

We are here faced with problems of the ordering fixation and of the inner product choice. However, as we have already obtained the unique orderings in the group quantization, take it as a standard. Let us concentrate only on the following two reasonable choices (both of which yield the same result as Eq. (9), see Eq. (23) below):

Choice (a): *Taking the Cartesian coordinates as a guidance.*

We regard that the Cartesian expression

\[
\begin{aligned}
  C_{\text{cart}} &= -\frac{\hbar^2}{2m} (\partial_x^2 + \partial_y^2) - \frac{k}{\sqrt{x^2 + y^2}} - E,
  \\
  \text{inner product: } dxdy
\end{aligned}
\]

exists *prior* to the polar expression, and that the former has been transformed to the latter:
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\[ C_0 \psi(r, \theta) = \left\{ -\frac{\hbar^2}{2m} \left( \frac{1}{r} \partial_r r \partial_r + \frac{1}{r^2} \partial_\theta^2 \right) - \frac{k}{r} - E \right\} \psi(r, \theta) = 0 , \quad (16 \cdot a) \]

inner product: \( r^2 dr d\theta \).

Choice (b): Taking the symmetry of the phase space as a guidance.

We respect the symmetry \( SO(3) \) and find out the ordering which reproduces \( SO(3) \). In the present case we have already found out the ordering in the previous section. Performing the "simple replacement" \( p_\theta \rightarrow -i\hbar \partial_\theta \) in Eq. (6\cdot d), one obtains

\[ C_0 \phi(r, \theta) = \left\{ -\frac{\hbar^2}{2m} \partial_r^2 - \frac{\hbar^2}{2mr^2} \left( \partial_\theta^2 + \frac{1}{4} \right) - \frac{k}{r} - E \right\} \phi(r, \theta) = 0 , \quad (16 \cdot b) \]

inner product: \( dr d\theta \).

One should note that this choice (b) corresponds to the original Dirac's prescription. The classical Poisson bracket algebra should be preserved after quantization, otherwise the interpretation of the 1st class constraints as the postulation on the physical states would not be justified.

We should note that two choices (a) and (b) become equivalent to each other by the identification

\[ \psi(r, \theta) = r^{-1/2} \phi(r, \theta) . \]

In fact, substituting (17) into Eq. (16\cdot a), Eq. (16\cdot b) is obtained and (17) means

\[ \psi^* \phi_2 r dr d\theta = \phi^* \psi_2 dr d\theta . \]

It may be instructive to summarize the relation between (a) and (b) as follows:

classical constraint + ordering and inner product respecting for Cartesian coordinates

\( \Rightarrow \) constraint respecting for the symmetry + "simple" replacement and inner product.

Remembering this equivalence, we proceed discussions below by the choice (b).

Now, normalizing \( r \) and \( E \) as

\[ \rho := r/R_{\text{Bohr}} = r/\sqrt{\frac{\hbar^2}{km}} , \quad \frac{1}{n^2} := E/\frac{k}{2R_{\text{Bohr}}} \]

and putting \( \phi(r, \theta) = \chi(\rho) e^{i\theta} \), one obtains

\[ \frac{d^2}{d\rho^2} \chi + \left( -\frac{1}{n^2} + \frac{2}{\rho} - \frac{l^2 - 1/4}{\rho^2} \right) \chi = 0 . \]

Let us solve Eq. (18) by investigating the asymptotic behaviors of solutions, when \( \rho \rightarrow 0 \) and \( \rho \rightarrow \infty \).

1. The behavior when \( \rho \rightarrow 0 \). Putting \( \chi(\rho) = \rho^l (1 + \rho \lambda + \cdots) \) and substituting it into Eq. (18), \( \lambda \) is determined as \( \lambda = l + 1/2 \) or \( -(l - 1/2) \). Thus, solutions regular when \( \rho \rightarrow 0 \) behave as

\[ \chi(\rho) \sim \rho^{l+1/2} \] (19\cdot a)
and \( l \) should be at least \( l+1/2 > 0 \), which will be discussed further below.

(2) The behavior when \( \rho \to \infty \). When \( \rho \to \infty \), Eq. (18) becomes roughly \((d^2/d\rho^2)\chi \sim (1/n^2)\chi\), and so \( \chi \sim e^{-(\rho/n)} \). Putting \( \chi(\rho) = e^{-(\rho/n)}\rho^\nu \) and substituting it into Eq. (18), one finds that \( \nu = n \). Thus,

\[
\chi(\rho) \sim e^{-(\rho/n)}\rho^n. \tag{19·b}
\]

(3) Considering the asymptotic behaviors (19·a, b), one puts \( \chi(\rho) = \rho^{l+1/2}W(\rho)e^{-(\rho/n)} \) and substitutes it into Eq. (18). Then \( W(\rho) \) turns out to be a function which obeys the following differential equation:

\[
x^2 \frac{d^2 W}{dx^2} + \left[(2l+1) - x^2\right] \frac{dW}{dx} - (l + 1/2 - n) W = 0,
\]

where \( x := (2/n)\rho \).

The solution of this equation can be represented by the confluent hypergeometric function \( F(-n + l + 1/2, 2l + 1; x) \).

One has finally obtained the solution of Eq. (18) which are regular when \( \rho \to 0 \) and \( \rho \to \infty \):

\[
\phi(\rho, \theta) = \sum c_i \rho^{l+1/2} F\left(-n + l + 1/2, 2l + 1; \frac{2n}{\rho}\right) e^{-(\rho/n)}e^{i\theta}, \tag{20}
\]

where the \( c_i \) are some constants. We note here that the form of solutions (20) reflects the number of space dimension. Above all, the last term \( e^{i\theta} \) would be replaced by \( Y_m(\theta, \phi) \) if the space dimension were three.

Next, let us examine the well-definedness of the operator \( \hat{C} \), and find out the allowed values of \( l \). Consider the operators \((d^2/d\rho^2)\) and \((1/\rho^2)\) in (18). From the postulation of convergence of \( \int_0^\infty \phi^* d\phi \), \( \int_0^\infty \rho^2 \phi^* (d^2/d\rho^2) \phi \, d\rho \), and the hermiticity of \((d^2/d\rho^2)\) (noting that \( \int_0^\infty \phi^* (d^2/d\rho^2) \phi \, d\rho = \int_0^\infty (d^2/d\rho^2) \phi^* \phi \, d\rho \)), \( \phi \) should satisfy

\[
\phi \sim O(\rho^{1/2+\varepsilon}), \tag{21·a}
\]

\[
\phi \sim O\left(\frac{1}{\rho^{1/2+\varepsilon}}\right), \tag{21·b}
\]

where \( \varepsilon, \varepsilon' > 0 \).

Comparing these restrictions with (19·a, b), one finds out that \( l \) should not be a negative number. Because the case \( l=0 \) is marginal, examine this case further.

When \( l=0 \), \((d^2/d\rho^2)\) and \((1/\rho^2)\) enter into \( \hat{C} \) in Eq. (18) only by the combination of \((d^2/d\rho^2) + (1/4)(1/\rho^2)\). Thus \( \int \phi^* (d^2/d\rho^2) + (1/4)(1/\rho^2) \phi \, d\rho \) behaves like \( (\lambda - (1/2))^2 \times \int \rho^{2l-2} \, d\rho \) when \( \phi \sim \rho^l \) near \( \rho \sim 0 \). Thus the allowed region of \( \lambda \) is \( \lambda \geq 1/2 \), and the value \( l = 0 \) is therefore allowed. Hence \( l \) should be

\[
l \geq 0. \tag{22}
\]

Now, let us examine the restriction on the number \( n \). Because the first argument of the confluent hypergeometric function \( F \) in Eq. (20) should be 0 or a negative
integer for regularity,
\[-n + l + 1/2 = 0, -1, -2, \ldots,\]
or
\[n = l + 1/2, \ (l + 1) + 1/2, \ (l + 2) + 1/2, \ldots.\]

In other words, because \( E = -\frac{mk^2}{2\hbar^2} (1/n^2) \), \( E \) should be
\[E_j = -\frac{mk^2}{2\hbar^2} \frac{1}{(j + 1/2)^2}. \ (j = l, l + 1, \ldots) \quad (23)\]

Here we are faced with a problem specific to the Dirac-Wheeler-DeWitt method: One must further postulate a certain periodicity of states with respect to the variable \( \theta \) in order to determine the allowed values of \( l \), and accordingly, \( j \). In usual cases, we know the geometrical meaning of \( \theta \) from the outset and postulate the single-valuedness (or double-valuedness) of states, obtaining \( l = 0, 1, 2, \ldots \) (or \( l = 1/2, 3/2, 5/2, \ldots \)). However, looking at our constrained system \( ((r, p_r), (\theta, p_\theta); C = (p_r^2/2m) + (p_\theta^2/2mr^2) - (k/r) - E = 0) \) without any preliminary knowledge or prejudice, there is no a priori reason for the periodicity of states with respect to \( \theta \). (This is also related to the ambiguity in the measure. There is no a priori reason for the integral region of \( \theta \) to be from 0 to 2\( \pi \).)

On the contrary, one obtains a rigorous and decisive restriction on this point in the group quantization method. Given a constrained system \( ((r, p_r), (\theta, p_\theta); C = (p_r^2/2m) + (p_\theta^2/2mr^2) - (k/r) - E = 0) \) without any preliminary knowledge, one may be lucky enough to find out that the \( \mathcal{U} \)'s, the classical version of the expressions \( (4 \cdot a \sim c) \), are physical observables and that they define the \( SU(2) \) Poisson bracket algebra. For the construction of the representation, \( J = 0, (1/2), 1, (3/2), 2, (5/2), 3, \ldots \) (with inner product between states also determined).

This observation tells us that, in some cases, the group-quantization point of view provides us some facts which otherwise were hard to be known.

§ 6. Construction of the generalized models

One can construct other models, which describe some series of Hamiltonian vanishing systems, by the natural generalization of our model, which is based on the \( SU(2) \sim SO(3) \) symmetry of \( S_{\text{phys}} \).

In the language of Lie algebra, what we have done so far can be reexpressed and generalized as follows:

1. Take a certain Lie algebra \( \mathcal{G} \). (Let \( \dim \mathcal{G} = N \), rank \( \mathcal{G} = r \).)
2. Noting that the number of the Casimir operators in \( \mathcal{G} \) is equal to rank \( \mathcal{G} = r \) by Racah's theorem, construct \( r \) constraint operators as \( \tilde{C}_1 = h_1(\tilde{\gamma}_1), \tilde{C}_2 = h_2(\tilde{\gamma}_2), \ldots, \tilde{C}_r = h_r(\tilde{\gamma}_r) \), where \( \tilde{\gamma}_1, \tilde{\gamma}_2, \ldots, \tilde{\gamma}_r \) are the Casimir operators and \( h_1, h_2, \ldots, h_r \) are suitably chosen functions.
The corresponding classical constrained system is
\[(S; C_1 \approx 0, C_2 \approx 0, \ldots, C_r \approx 0)\]
s.t. \[3 \mu_i's \in C^\infty(S, \mathbb{R}) \ (i=1, 2, \ldots, N)\]

obey the Poisson bracket algebra corresponding to \( \mathcal{G} \).
\((C_k's \in C^\infty(S, \mathbb{R}) \ (k=1, 2, \ldots, r)\) are classical analogues of \( \mathcal{C}_k \).

Note that \( \dim S \) should be \( N + r \). Regarding (2), the function \( h_k's \) should be chosen so that they have zeros at (at least some subset of) the eigenvalues of \( \mathcal{F}_k \) allowed by the representation theory of \( \mathcal{G} \).

Our model corresponds to \( \mathcal{G} = \text{su}(2) \approx \text{so}(3) \), so that \( N = 3, r = 1 \). Let \( \bar{\nu}_1, \bar{\nu}_2, \bar{\nu}_3 \) be the usual non-dimensional generators. The Casimir operator is thus \( \bar{\mathcal{F}} = \bar{\nu}_1^2 + \bar{\nu}_2^2 + \bar{\nu}_3^2 \). One possibility for the constraint operator is \( \bar{C}' = a \bar{\mathcal{F}} - b \) (corresponding to \( (1/|E|) (\bar{u}_a^2 + (1/4) \hbar^2) \bar{C} \) in our model, see Eq. (7)), where \( b/a \) should be \( J(J+1)(J=0, 1/2, 1, 3/2, 2, \ldots) \).

For \( \mathcal{G} = \text{so}(4) \), which is related to the 3-dimensional Kepler model, \( N = 6 \) and \( r = 2 \). One can choose six generators \( (\bar{\nu}_1, \bar{\nu}_2, \bar{\nu}_3, \bar{\omega}_1, \bar{\omega}_2, \bar{\omega}_3) \) such that two Casimir operators are expressed as
\[ \mathcal{F}_1 = \bar{\nu}^2 + \bar{\omega}^2, \quad \mathcal{F}_2 = \bar{\nu} \cdot \bar{\omega} \]

One can choose as
\[ \bar{C}_1 = a \bar{\mathcal{F}} - b, \quad \bar{C}_2 = c \bar{\mathcal{F}} - d. \]

The usual Kepler system (or the model for a hydrogen atom) can be regarded as a special case \( d = 0 \) (see Eq. (2·a)). Given a certain Lie algebra \( \mathcal{G} \), one can straight­forwardly construct a model suitable for the group quantization by the above pre­scription (2). For example, \( \mathcal{G} = \text{so}(n, m) \) is the most natural extension of our original model. The problem is (3): It is in general difficult to find out explicitly the setting-up phase space \( S \), in terms of which the physical interpretation may be easier.

There are two more remarks:

1°) As is well known, one of the Casimir operators for \( \mathcal{G} \) is expressed as a bilinear form of generators. The constraint operator corresponding to this is likely to be at a physically special position relative to the other constraint operators. Indeed, in our Kepler model, it is deeply connected with the Hamiltonian in a usual sense.

2°) (1)~(3) are the general features for any Hamiltonian-vanishing systems to be subject to the group quantization scheme. The above point of view, i.e., to look upon the constraints as functions of Casimir operators of some algebra, might be useful also for gravity.

§ 7. Discussion

Let us compare the group quantization method and the Dirac-Wheeler-DeWitt method taking the Kepler model as an example. The main point, can be summarized as follows:
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<table>
<thead>
<tr>
<th>Procedure</th>
<th>Group quantization</th>
<th>Dirac-Wheeler-DeWitt method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantized variables</td>
<td>• Finding out a symmetry group $G$ → unitary representation</td>
<td>• Solving the Wheeler-DeWitt equation with suitable boundary conditions.</td>
</tr>
<tr>
<td></td>
<td>• Physical observables</td>
<td>• Need for finding out the ordering which reproduces $G$.</td>
</tr>
<tr>
<td></td>
<td>$f_i$, s.t. $(f_i, C)_M \approx 0$</td>
<td>• Need for finding out the ordering and the inner product (some &quot;natural&quot; choices exist, but not decisive.).</td>
</tr>
<tr>
<td></td>
<td>${f_i, f_j}<em>M = c</em>{ij} f_k$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>${f_i, f_j} = i \hbar c_{ij} f_k$</td>
<td></td>
</tr>
<tr>
<td>State vectors</td>
<td>• The representation space for $G$</td>
<td>• Canonical variables ${(q, p)_M \rightarrow [q, p] = i \hbar}$</td>
</tr>
<tr>
<td></td>
<td>$\langle f</td>
<td>\sum M c^M</td>
</tr>
<tr>
<td>The relation between states and observations</td>
<td>• Difficult to understand</td>
<td>• Easier</td>
</tr>
<tr>
<td>The operator orderings</td>
<td>• Almost unique</td>
<td>• The arguments of states are canonical variables so that physical observables are not respected.</td>
</tr>
<tr>
<td>The spectrum $E_J$ (proper to the Kepler model)</td>
<td>• Not easy to find out (even for the Kepler model).</td>
<td>• Ambiguity exists (Some &quot;natural&quot; choices exist for some models).</td>
</tr>
<tr>
<td></td>
<td>$E_J = -E e^{(J+1/2)^2}$</td>
<td>$E_J = -E e^{(J+1/2)^2}$</td>
</tr>
<tr>
<td></td>
<td>$J = 0 \quad 1 \quad 2 \quad \ldots$</td>
<td>$\ldots$</td>
</tr>
<tr>
<td></td>
<td>$1 \quad 2 \quad 3 \quad 5 \quad \frac{1}{2}$</td>
<td>$1 \quad 2 \quad 3 \quad 5 \quad \frac{1}{2}$</td>
</tr>
<tr>
<td></td>
<td>$\ldots$</td>
<td>$\ldots$</td>
</tr>
</tbody>
</table>

We have so far examined the group quantization method using a simple, non-trivial model, the Kepler model. Since this model has the adequate physical contents, in spite of its simplicity, it will serve as a preliminary toy-model for the investigation of the group quantization of constrained systems.

According to our above considerations on the group quantization with the Kepler model, purely algebraic contents, e.g., state vectors and the inner product on them, are uniquely determined through the symmetry group $G$ and its representation. However, the other physically significant contents, e.g., the "energy spectrum" (the allowed values of the parameter $E$), have never been obtained until one specifies the correct operator ordering.

The physical observables are quantized in this method, which is a reasonable treatment for constrained systems. The interpretation of wave functions, however, is difficult because the arguments of wave functions are eigenvalues of physical observables, not canonical variables which one has chosen at the beginning. This difficulty is also connected with the difficulty of setting boundary conditions to determine the coefficient $c^M$s in Eq. (10). It may be in general more difficult to express natural
boundary conditions in terms of physical variables than in terms of canonical variables.

On the other hand, the Dirac-Wheeler-DeWitt method has also conceptual difficulties. The fundamental canonical variable $r$ is not a physical observable $(\langle r, C \rangle_{PB} \neq 0)$ ($r$ is analogous to the scale factor $a$ of the universe, in the quantum cosmological context). This means physically that $r$ can never be observed (if $r$ had been observed, the phase point would have been kicked out of the constraint surface). In spite of this fact, in the Dirac-Wheeler-DeWitt method, one solves the differential equation with respect to $r$ with suitable boundary conditions expressed in terms of $r$ (in addition to the regularity conditions such as the asymptotic behavior of $\phi$ when $r \to 0$ or $r \to \infty$).

Thus, we must answer the following questions:

1. Is it meaningful to set up boundary conditions in terms of $r$?
2. How do we relate $\phi(r)$ with observations?

It may be that we should pay more attention in quantum cosmology to the diffeomorphism invariant quantities, such as the total volume or the global topology of the space-time, rather than operationally convenient quantities, such as the scale factor $a$.

Another possible approach is to study the states obtained by the group quantization, such as $|J\rangle$, in terms of the canonical variables like $r$. Such a kind of investigation, however, is not so easy because the relation between the physical observable $u_i$'s and the canonical variables $(\langle r, p_r \rangle, (\theta, p_\theta))$ are non-trivial and complicated.

It can be at least said that the group quantization method provides us one useful viewpoint to the constrained systems and that it also gives many suggestions for the Dirac-Wheeler-DeWitt method.

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