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Discrete spectrum of the hydrogen atom: an illustration of deformation theory methods and problems

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0. INTRODUCTION

This paper reproduces part of the content of three lectures delivered by us at the S. Banach Institute in November 1983, during the semester of Mathematical Physics. We have omitted here the general review of deformation theory which we gave, as this can be found without difficulty in the literature [i.e. 1, 2, 7].

Bayen et al [1] have proposed to build quantum mechanics on «classical» phase space, i.e. a symplectic manifold, with «classical» observables, i.e. functions on that manifold; quantization arises as a deformation called a $*$ product of the algebra of functions. In this approach, one avoids the usual setting of self adjoint operators on a Hilbert space, and one gets a unified framework of both classical and quantum mechanics; in particular, it allows an easy interpretation of the fact that classical mechanics is a limit of quantum mechanics when the Planck constant tends to zero.

In this deformation approach, Bayen and al have defined the notion of spectrum of an observable; their definition is given entirely in terms of $*$ product. In particular, they have computed the specturm of the hydrogen atom [1], in a completely intrinsic $*$ product way.

We discuss here the Kepler problem again, from a different point of view. The main difference is that we define a generalized Weyl transform; this implies that we use operators for our computation of spectra. The Weyl transform (§2 and §4) is directly related to the $*$ product and to the group $SO(4)$ of invariance of the problem. The construction and the properties of such a correspondence

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for non abelian groups have independent interest.

One other aspect of this paper is that we compute the spectrum with two different mathematically equivalent $*$ products; one is induced by Moyal product on $\mathbb{R}^8$ - this was the one introduced and used in [1] - and the other is given intrinsically on the cotangent bundle to an arbitrary Lie group. It is not surprising that we get different spectra; indeed, already for $\mathbb{R}^{2n}$ different orderings correspond to mathematically equivalent $*$ products and as is well known different orderings in quantum mechanics usually lead to different spectra.

We feel that the «quantization choice» made by physics should be analyzed in greater details, and lead to restrictions on the class of $*$ products on one hand and to the notion of spectral equivalence for deformations on the other hand. In particular, it is remarkable that physics chooses the Moyal $*$ product (i.e. symmetric ordering) which is intrinsically characterized on $\mathbb{R}^{2n}$ by a maximal invariance property. In this direction, the invariance (or more precisely the covariance) of the $*$ products considered here under $SO(4, 2)$ should be investigated.

The paper is organized as follows. In § 1 we exhibit the regularisation of the Kepler problem as given by J.-M. Souriau [10]. Classical phase space is an open submanifold of the cotangent bundle to the group $SU(2)$. This is not the regularisation used in [1]. It has the drawback that it corresponds only to the bound states (i.e. discrete spectrum); on the other hand it is geometrically very beautiful. In § 2, we recall the definition of $*$ product, mathematical equivalence, invariance and - in the framework of $\mathbb{R}^{2n}$ - Weyl correspondence. This is used to give a $*$ notion of spectrum, equivalent to the one given in [1]. The § 3 is devoted to recall the explicit construction of two different $*$ products on the cotangent bundle to $SU(2)$, both invariant under $SO(4)$. Finally § 4 contains the generalized Weyl transform and two computations of the spectrum.

During the preparation and the redaction of this paper we had innumerable discussions with our friends M. Flato and D. Sternheimer; they have enormously contributed to the clarification of the notions used here; we thank them wholeheartedly.

1. REGULARISATION OF THE KEPLER PROBLEM [10]

The Kepler problem is the classical mechanics description of a point particle in a central attractive force field, the intensity of which is inversely proportional to the square of the distance of that particle to the attractive center. If $\bar{r}$ denotes the position of the particle in a Galilean frame attached to the center and if $\bar{v}$ is its velocity, the differential equations governing the motion are:

$$\frac{\mathrm{d}\bar{r}}{\mathrm{d}t} = \bar{v}$$

$$\frac{\mathrm{d}\bar{v}}{\mathrm{d}t} = -\frac{\bar{r}}{r^3} \qquad (r \underset{\text{def}}{=} \|\bar{r}\|).$$

The well known constants of the motion are:

(i) the energy $E = \frac{1}{2}\bar{v}^2 - \frac{1}{r}$. We shall assume from now on that $E < 0$.

(ii) the angular momentum $\bar{\hbar} = \bar{r} \wedge \bar{v}$

(iii) the Lenz vector $\bar{L} = \frac{1}{\sqrt{-2E}}\left[\bar{\hbar} \wedge \bar{v} + \frac{\bar{r}}{r}\right]$.

The evolution space of this system is the open subset of $\mathbb{R}^7$, $\mathcal{E} = \{(\bar{r}, \bar{v}, t) \mid E < 0, r \neq 0\}$; the fundamental vector field is:

$$Z = \bar{v}\,\partial_{\bar{r}} - \frac{\bar{r}}{r^3}\,\partial_{\bar{v}} + \partial_t .$$

An equivalence relation is defined on $\mathcal{E}$ by $x \sim y$ if x and y belong to the same integral curve of Z or to the same «extended» integral curve of Z. If $H = 0$, the motion leads to collision after a finite time, the integral curve of Z is extended in the future by taking its «mirror image» with respect to the instant of collision preserving energy and trajectory; it is similarly extended in the past before the moment of an «initial collision» by taking a «mirror image». Let p denote the canonical projection $\mathcal{E} \to \mathbb{K} = \mathcal{E}/_{\sim}$; a smooth manifold structure is defined on $\mathbb{K}$ by a collection of charts (C_j, φ_j) where $C_j = \{k \in \mathbb{K} \mid k$ has no collision at time $t_j\}$ and $\varphi_j : C_j \to \mathbb{R}^6 : (\bar{r}, \bar{v}, t) \to (\bar{r}_{t_j}, \bar{v}_{t_j})$. This manifold $\mathbb{K}$ is the phase space of the Kepler problem.

The symplectic structure Ω in $\mathbb{K}$ is defined as follows, let β be the 1-form on $\mathcal{E}$:

$$\beta = \bar{v}\,\mathrm{d}\bar{r} - E\,\mathrm{d}t + \mathrm{d}(3Et - 2\bar{r}\cdot\bar{v}).$$

One checks that

$$i(Z)\beta = 0 = L_Z\beta.$$

There exists thus a 1-form $\tilde{\beta}$ on $\mathbb{K}$ such that $\beta = p^*\tilde{\beta}$. We then define

$$\Omega = \mathrm{d}\tilde{\beta}.$$

Souriau has shown that $(\mathbb{K}, \Omega)$ is naturally symplectomorphic to the cotangent bundle to the 3-sphere T^*S^3, with its canonical symplectic form, from which one has deleted the zero section. We simply recall here the pertinent definitions.

The cotangent bundle T^*S^3 is considered as a submanifold of $\mathbb{R}^8 = T^*\mathbb{R}^4 = \mathbb{R}^4 \times \mathbb{R}^{4*}$. More precisely

$$T^*S^3 = \{(Q,P) \in \mathbb{R}^4 \times \mathbb{R}^{4*} \mid Q^2 = 1, \langle P, Q\rangle = 0\}.$$

Let us define a map $q_0 : \mathcal{E} \to T^*S^3$; denote by $(A,B)(\bar{r},\bar{v},t)$ the (4×2) matrix:

$$(A,B) = \begin{pmatrix} (\bar{r}\cdot\bar{v})\,\bar{v} - \dfrac{\bar{r}}{r} & 2Er\bar{v} \\ \bar{r}\cdot\bar{v} & 2Er+1 \end{pmatrix}$$

and let

$$(P_0,Q_0) = \begin{pmatrix} \dfrac{1}{\sqrt{-2E}} I_3 & 0 \\ 0 & 1 \end{pmatrix} (A,B) \begin{pmatrix} \cos\sqrt{-2E}(\bar{r}\cdot\bar{v}-2Et) & \sqrt{-2E}\sin\sqrt{-2E}(\bar{r}\cdot\bar{v}-2Et) \\ -\dfrac{1}{\sqrt{-2E}}\sin\sqrt{-2E}(\bar{r}\cdot\bar{v}-2Et) & \cos\sqrt{-2E}(\bar{r}\cdot\bar{v}-2Et) \end{pmatrix}$$

then $q_0(\bar{r},\bar{v},t) = (Q_0,P_0)$. One checks that $q_0 : \mathcal{E} \to T^*S^3$ factorizes through $\mathbb{K}$, and that the induced map $\bar{p}_0 : \mathbb{K} \to T^*S^3$ is a symplectic diffeomorphism if one deletes the zero section and if the symplectic form on T^*S^3, is the restriction to T^*S^3 of the symplectic form on $T^*\mathbb{R}^4$, $-\mathrm{d}P_0 \wedge \mathrm{d}Q_0$. The absence of the zero section is justified by the fact that:

$$P_0^2 = -\frac{1}{2E}\,.$$

We will from now on identify $\mathbb{K}$ with $T^*S^3 \setminus \{\text{zero section}\}$; the hamiltonian function H on $\mathbb{K}$ is the energy function E, which is the restriction of the function $-\dfrac{1}{2P^2}$. The functions associated to the constants of the motion $\bar{h}$ and $\bar{L}$ are respectively:

$$\bar{h} = (\bar{P}\wedge\bar{Q})|_{T^*S^3}, \qquad (\bar{P},\bar{Q} = 3 \text{ vectors corresponding to the first 3 components of } P, Q).$$

$$\bar{L} = (Q_4\bar{P} - P_4\bar{Q})|_{T^*S^3}\,.$$

One recognizes the 6 functions on T^*S^3, which are induced on this symplectic manifold, by the usual lift to T^*S^3 of the standard action of $O(4)$ on $S^3 \subset \mathbb{R}^4$.

It is useful to observe that the hamiltonian H does not belong to the universal envelopping algebra $\mathfrak{U}\,(so(4))$ which can be identified to the vector space of restrictions to T^*S^3 of polynomials in the functions $P \wedge Q$; on the other hand H^{-1} does belong to $\mathfrak{U}(so(4))$.

2. GENERALITIES ON $*$ PRODUCTS

Let (M, F) be a smooth $2n$-dimensional symplectic manifold and let $N = \mathbb{C}^\infty(M, \mathbb{C})$; denote by $E(N, \nu)$ the space of formal power series in $\nu (\in \mathbb{C})$ with coefficients in N.

DEFINITION 1. *A* $*$ product *on* (M, F) *is a bilinear map* $N \times N \to E(N; \nu)$. $(f, g) \to f * g = \sum_{r=0}^{\infty} \nu^r C_r(f, g)$ which satisfies the following axioms:

(i) $C_0(f, g) = f \cdot g$

(ii) $C_1(f, g) = \{f, g\} =$ *Poisson bracket of* f *and* $g = F(X_f, X_g)$ *where* $X_f(X_g)$ *is defined by* $i(X_f)F = -\mathrm{d}f$, $(i(X_g)F = -\mathrm{d}g)$

(iii) $C_r(f, g) = (-1)^r C_r(g, f)$

(iv) $(f * g) * h = f * (g * h)$; *this has a meaning as* $*$ *extends in an obvious way to a bilinear map* $E(N, \nu) \times E(N; \nu) \to E(N, \nu)$

(v) $\forall r \geqslant 1$, C_r *is a bidifferential operator vanishing on the constants.*

REMARKS. (a) A $*$ product is, by virture of (i) and (iv), a formal deformation of the associative structure of N.

(b) If ν is pure imaginary, $\overline{f * g} = \bar{g} * \bar{f}$ by virture of (iii)

(c) $\dfrac{1}{2\nu}(f * g - g * f) = \sum_{r=0}^{\infty} \nu^{2r} C_{2r+1}(f, g)$ is by virture of (ii) and (iv) a formal deformation of the Lie algebra structure of N, given by the Poisson bracket.

DEFINITION 2. *Two star products on* (M, F), $*$ *and* $*'$ *are said to be* mathematically equivalent *if there exists a formal power series*

$$\mathfrak{T} = \sum_{r=0}^{\infty} \nu^r T_r$$

where T_r *is a linear map* $N \to N$ *given by a differential operator and where* T_0 *is the identity map, such that for all* $f, g \in N$ *one has:*

$$\mathfrak{T}(f * g) = \mathfrak{T}f *' \mathfrak{T}g.$$

PROPOSITION 1. [8] *If the second de Rham cohomology group of* M *vanishes, all* $*$ *products on* M *are mathematically equivalent.*

Let G be a Lie group of symplectomorphisms of (M, F) and let $\mathfrak{g}$ be the Lie algebra of G. If $X \in \mathfrak{g}$, the vector field X^* on M associated to X has for value at the point $x \in M$:

$$X_x^* = \frac{\mathrm{d}}{\mathrm{d}t}(\exp - tX \cdot x)_{t=0}.$$

The action of G on M is hamiltonian if, for all $X \in \mathfrak{g}$, there exists a function $f_X \in N$ such that

$$i(X)F = -\,\mathrm{d}f_X$$

and if furthermore, for all $X, Y \in \mathfrak{g}$,

$$\{f_X, f_Y\} = f_{[X,Y]}.$$

DEFINITION 3. *A $*$ product on (M, F) is said to be G* geometrically invariant *if for all $f, g \in N$ and for all $k \in G$*

$$k^*(f * g) = (k^*f) * (k^*g).$$

A $*$ product on (M, F) is called a $*$ representation of $\mathfrak{g}$ *if for all $X, Y \in \mathfrak{g}$,*

$$\frac{1}{2\nu}(f_X * f_Y - f_Y * f_X) = \{f_X, f_Y\} = f_{[X,Y]}.$$

When both these invariance conditions are satisfied the $*$ product is said to be strongly invariant *by G.*

PROPOSITION 2. [6] *If the second G-invariant de Rham cohomology group of M vanishes and if there exists on M a G-invariant connection, two G geometrically invariant star products, $*$ and $*'$ are invariantly equivalent, i.e. the formal power series $\mathfrak{T}$ defining the equivalence can be chosen such that the T_r's are G invariant differential operators.*

Example: The Moyal $*$ product is defined on $\mathbb{R}^{2n}$, which is identified with the cotantent bundle to the abelian group $\mathbb{R}^n$; the symplectic structure F is the standard one on $T^*\mathbb{R}^n$. We shall denote by q^i $(i \leqslant n)$ the coordinates on $\mathbb{R}^n$ and, with a little abuse of notation, by (q^i, p_i) the coordinates on $T^*\mathbb{R}^n$. In these coordinates, the symplectic form F reads:

$$F = \sum_{i=1}^{n} \mathrm{d}p_i \wedge \mathrm{d}q^i.$$

The affine symplectic group $\mathbb{R}^{2n}$, $G = Sp(n, \mathbb{R}) \cdot \mathbb{R}^n$, has a hamiltonian action on $T^*\mathbb{R}^n$.

Let $F = \begin{pmatrix} 0 & -I_n \\ I_n & 0 \end{pmatrix}$ be the matrix associated to the symplectic form and let $\Lambda = \begin{pmatrix} 0 & -I_n \\ I_n & 0 \end{pmatrix} = -F^{-1}$; the elements of Λ are designated by Λ^{ab} $(a, b \leqslant 2n)$.

The Moyal $*$ product is defined on N by:

$$f * g = fg + \sum_{r=1}^{\infty} \frac{\nu^r}{r!} P_r(f, g)$$

$$P_r(f, g) = \sum_{\substack{a_1 \ldots a_r \\ b_1 \ldots b_r}=1}^{2n} \Lambda^{a_1 b_1} \ldots \Lambda^{a_r b_r} \partial^r_{a_1 \ldots a_r} f \, \partial^r_{b_1 \ldots b_r} g.$$

It is clearly G invariant in the strong sense and it can be shown that this invariance property uniquely characterizes the Moyal product.

The function p_i is the function corresponding to the element ∂_{q^i} of the Lie algebra of $\mathbb{R}^n$; the injective Lie homomorphism $\mathbb{R}^n \to N$ which sends ∂_{q^i} on p_i «extends» to an associative injective homomorphism of $\mathfrak{U}(\mathbb{R}^n)$ (= the universal envelopping algebra of $\mathbb{R}^n$) $\to N$; the image of this homomorphism is the associative algebra of polynomials in the variables p_i's with constant coefficients. We shall be concerned with the associative algebra A of polynomials in the p_i's with coefficients which are smooth functions of the q^i's ($A = \{h : \mathbb{R}^n \to \mathfrak{U}(\mathbb{R}^n) \mid$ smooth$\}$) and with the subalgebra B of polynomials in the p_i's with coefficients which are polynomials in the q^i's. Both A and B are also associative algebras with respect to the Moyal $*$ product.

In the classical formulation of quantum mechanics one associates to each function on $\mathbb{R}^{2n}$ belonging to a certain class, a self adjoint operator on $L^2(\mathbb{R}^n)$; in particular to the «position» q^j corresponds the operator $q^j \cdot I$ and to the momentum p_j corresponds the operator $\frac{\hbar}{i} \partial_{q^j}$ $\left(\hbar = \frac{1}{2\Pi} \times \text{Planck constant}\right)$. One way to extend this into a linear map of B into the self adjoint operators on $L^2(\mathbb{R}^n)$ is to send a polynomial in p_j's and q^j's onto the corresponding completely symmetric expression in the elementary operators $q^j \cdot I$ and $\frac{\hbar}{i} \partial_{q^j}$. This correspondence has been generalized by Weyl to include non polynomial type functions; the domain of this generalized correspondence has been very extensively studied [4].

DEFINITION 4. *The* Weyl correspondence W *is the associative algebra homorphism* $(A, *) \to (\mathbf{A}, 0)$ (= *algebra of self-adjoint operators on* $L^2(\mathbb{R}^n)$) *such that* $W(q^j) = q^j I$ *and* $W(p_j) = 2\nu\partial_{q^j}$.

REMARK. We shall also use term Weyl correspondence for the extension of W to non polynomial functions in the variables p_i's, when we will deal with this extension we will remain formal in the sense that the domain of W is not made precise.

PROPOSITION 3. *The Weyl correspondence restricted to the* $*$ *algebra* B *sends a polynomial on the corresponding completely symmetrized operator.*

Proof. Assume first we have a polynomial of degree 1 in the p_j's. Then

$$W(p_i q^{i_1} \ldots q^{i_n}) = W\left(p_i * q^{i_1} * \ldots * q^{i_n} - \nu \sum_{j=1}^{n} \delta_i^{i_j} q^{i_1} \ldots \hat{q^{i_j}} \ldots q^{i_n}\right)$$

$$= 2\nu\partial_i \circ q^{i_1} \circ \ldots \circ q^{i_n} - \nu \sum_{j=1}^{n} \delta_i^{i_j} q^{i_1} \circ \ldots \circ \hat{q^{i_j}} \circ \ldots \circ q^{i_n}$$

$$= \nu \sum_{j=1}^{n} \delta_i^{i_j} q^{i_1} \circ \ldots \circ \hat{q^{i_j}} \circ \ldots \circ q^{i_n} + 2\nu q^{i_1} \circ \ldots \circ q^{i_n} \partial_i.$$

On the other hand the completely symmetrized operator reads:

$$\frac{2\nu}{(n+1)!} \sum_{j=0}^{n} \sum_{\sigma \in S_n} q^{i_{\sigma(1)}} \ldots q^{i_{\sigma(j)}} \partial_i q^{i_{\sigma(j+1)}} \ldots q^{i_{\sigma(n)}}$$

and the two expressions are clearly equal. A completely parallel calculation shows that the equality also holds for a polynomial of degree 1 in the q^i's. By recurrence we can now assume that the equality holds on one hand for all degrees $< k$ in the variables p_j's and for these degrees in p_j's for all degrees in q^ℓ's and on the other hand for the degree k in p_j's and for all degrees $< n$ in q^ℓ's.

Observe then that one has the identity:

$$\sum_{\ell=1}^{k} p_{i_\ell} * (p_{i_1} \ldots \hat{p}_{i_\ell} \ldots p_{i_k} q^{j_1} \ldots q^{j_n}) + \sum_{m=1}^{n} q^{j_m} * (p_{i_1} \ldots p_{i_k} q^{j_1} \ldots \hat{q}^{j_m} \ldots q^{j_n}) =$$

$$2(p_{i_1} \ldots p_{i_k} q^{j_1} \ldots q^{j_n}).$$

Hence:

$$W(p_{i_1}\dots p_{i_k} q^{j_1}\dots q^{j_n}) = \frac{1}{k+1}\sum_{\ell=1}^{k} W(p_{i_\ell})\circ W(p_{i_1}\dots \hat{p}_{i_\ell}\dots p_{i_k} q^{j_1}\dots q^{j_n})$$

$$+\frac{1}{k+1}\sum_{m=1}^{n} W(q_{j_m})\circ W(p_{i_1}\dots p_{i_k} q^{j_1}\dots \hat{q}^{j_m}\dots q^{j_n})$$

which, by recurrence, is clearly the completely symmetrized operator.

Bayen and al. have given in [1] a $*$ product version of the Schrödinger equation and have suggested a definition for the spectrum of a hamiltonian function. We simply rephrase their definitions in a form which is going to be used in the applications we are making.

Let $\varphi : \mathbb{R}^n \to \mathbb{R}$ be a real analytic function and let ψ be the linear map defined by:

$$\langle \psi, f\rangle = (W(f)\varphi)(0) \qquad \forall f \in N \text{ for which } W(f) \text{ is defined.}$$

DEFINITION 5. *Given a hamiltonian function H on $\mathbb{R}^{2n}$ we define the corresponding* Schrödinger equation *as:*

$$\psi * H = E\psi$$

where E is a complex number and where $\psi * H$ is the linear map defined by

$$\langle \psi * H, f\rangle = \langle \psi, f * H\rangle \qquad \forall f \in N \text{ for which } W(f) \text{ is defined.}$$

REMARK. Using the definition of ψ we see that Schrödinger equation means that, for all appropriate functions f

$$(W(f)W(H)\varphi)(0) = E(W(f)\varphi)(0)$$

and in view of the analyticity of φ:

$$W(H)\varphi = E\varphi.$$

If one takes for hamiltonian function $H = \frac{1}{2}\sum_i p_i^2 + V(p)$ and $\nu = \frac{\hbar}{2i}$, this last relation is the usual Schrödinger equation.

DEFINITION 6. *The* spectrum *of the hamiltonian H is the set of complex numbers such that the corresponding Schrödinger equation admits a non trivial solution.*

3. STAR PRODUCTS ON T*S^3

The first $*$ product defined on T^*S^3 was described by Bayen and al. [1], we recall their construction.

We have shown in §1 that T^*S^3 appears naturally as symplectic submanifold of $T^*\mathbb{R}^4$ ($= \mathbb{R}^4 \times \mathbb{R}^{4*}$); it also appears naturally as a quotient of an open submanifold $\omega = \{(Q,P) \in T^*\mathbb{R}^4 \mid Q \neq 0\}$ by the group K (isomorphic to the connected component of the affine group of $\mathbb{R}$) acting on ω by:

$$(\rho, \sigma)(Q, P) = (\rho Q, \rho^{-1} P + \sigma Q) \qquad (\rho \in \mathbb{R}_0^+, \sigma \in \mathbb{R}).$$

This action of K on ω is clearly symplectic. Let $\Pi : \omega \to \omega/K$ be the canonical projection and let $\Pi' : \omega \to T^*S^3 (\subset T^*\mathbb{R}^4) : (Q,P) \to \left(\frac{Q}{\|Q\|}, \|Q\| P - \frac{\langle P, Q\rangle Q}{\|Q\|} \right)$; the map Π' factorizes throuth ω/K and one checks that the induced map $\alpha : \omega/K \to T^*S^3$ is a smooth diffeomorphism. The orbits of K in ω are 2-dimensional submanifolds; the tangent plane T at the point (Q,P) to the orbit of this point is spanned by the vectors:

$$X = Q\,\partial_Q - P\,\partial_P, \; Y = Q\,\partial_P.$$

The orbit is thus a symplectic submanifold of ω, furthermore there exists a 2-form γ of maximal rank on ω/K such that $\Pi^*\gamma|_{T^\perp} = -(\mathrm{d}P \wedge \mathrm{d}Q)|_{T^\perp}$ (where $T^\perp$ means the orthogonal to T relative to the symplectic form $\Omega \underset{\mathrm{def}}{=} -\mathrm{d}P \wedge \mathrm{d}Q$). The 2-form

$$\frac{1}{Q^2}\, i(X)\,\Omega \wedge i(Y)\Omega \underset{\mathrm{def}}{=} \lambda$$

is exact, vanishes identically on $T^\perp$ and is such that $\Omega(X, Y) = \lambda(X, Y)$. Hence

$$\Omega = \Pi^*\gamma + \lambda$$

and γ is a symplectic structure on ω/K.

The 2-form $\Pi'^*(-\mathrm{d}P \wedge \mathrm{d}Q|_{T^*S^3})$ is invariant by K, vanishes on the orbits; thermore $T^\perp$ at a point of T^*S^3 ($\subset T^*\mathbb{R}^4$) coincides with the tangent space to T^*S^3 at that point. Hence $\Pi'^*(-\mathrm{d}P \wedge \mathrm{d}Q|_{T^*S^3}) = \Pi^*\gamma$; as $\alpha \circ \Pi = \Pi'$ one concludes that:

$$\alpha^*(-\mathrm{d}P \wedge \mathrm{d}Q|_{T^*S^3}) = \gamma$$

and α is a symplectic diffeomorphism.

Let now $f, g \in N$ ($\omega/K = T^*S^3$) and denote by $\hat{f}(\hat{g}) = \Pi^*f(\Pi^*g)$. The Poisson bracket $\{\hat{f}, \hat{g}\}$ is a K invariant function on ω.

$$\{\hat{f}, \hat{g}\} = \mathrm{d}\hat{g}(X_{\hat{f}}) = \Pi^*(\mathrm{d}g(\Pi_* X_{\hat{f}})).$$

The vector field $X_{\hat{f}}$ is also K invariant, belongs to $T^\perp$, and

$$i(X_{\hat{f}})\Omega = -\,\mathrm{d}\hat{f} = -\,\Pi^*\mathrm{d}f = i(X_{\hat{f}})\Pi^*\gamma$$
$$= \Pi^*(i(\Pi_* X_{\hat{f}})\,\gamma).$$

Hence $\Pi_* X_{\hat{f}} = X_f$ and:

$$\{\hat{f}, \hat{g}\} = \widehat{\{f, g\}}.$$

This relation leads to a definition of a $*$ product on T^*S^3.

DEFINITION. *The «Moyal $*$ product» on T^*S^3 is defined by:*

$$\widehat{f * g} = \hat{f} * \hat{g} = \sum_{r=0}^{\infty} \frac{\nu^r}{r!}\, p^r(\hat{f}, \hat{g}).$$

Each term of the right hand side is a function on ω invariant by K as the P^r's are K invariant. The definition thus makes sense.

REMARK. All axioms of $*$ products, except axiom (v) are clearly satisfied. To check that the various terms are given by bidifferential operators it is enough to observe that a basis of vector fields on ω is given by $\{X, Y, Z_a(a \leqslant b)\}$ where $Z_a \in T^\perp$ and $[X, Z_a] = [Y, Z_a] = 0$. The invariance properties of the Moyal $*$ product imply that $P_r(\hat{f}, \hat{g})$ is expressed only in terms of Z_a derivatives of $\hat{f}$ and $\hat{g}$.

PROPOSITION 1. *The Moyal $*$ product on T^*S^3 is strongly invariant by the action of $O(4)$ on T^*S^3.*

Proof. Geometrical invariance of the $*$ product is obvious as the action of $O(4)$ on ω commutes with the action of K on ω and as $O(4)$ preserves the Moyal $*$ product. It is also a representation of $so(4)$ because the functions $P \wedge Q\,|_{T^*S^3}$ are the functions associated to a basis of $so(4)$ and because $\widehat{P \wedge Q}\,|_{T^*S^3} = P \wedge Q$.

One can identify $SU(2)$ to S^3 by considering the point $(\alpha, \beta) \in \mathbb{C}^2$ $(|\alpha|^2 + |\beta|^2 = 1)$ as a point in $\mathbb{R}^4$. The left action of $SU(2)$ on itself, lifts to an action of $SU(2)$ on T^*S^3 which is hamiltonian. We shall call $\tilde{p}_i$ $(i \leqslant 3)$ the functions corresponding to this action and one checks that

$$\tilde{p}_i = h_i - L_i \qquad \text{(cf. §1).}$$

Similarly if we denote by p_i the functions corresponding to the «right action» of $SU(2)$ on T^*S^3 one has

$$p_i = h_i + L_i.$$

In addition the p_i are quadratic functions on $T^*\mathbb{R}^4$ and one checks that:

$$p_i * p_j = p_i p_j + \nu\{p_i, p_j\} + 4\nu^2\delta_{ij}.$$

The second $*$ product on T^*S^3, is the intrinsic $*$ product defined by identifying T^*S^3 to $T^*SU(2)$. Let G be an arbitrary Lie group, let us denote by T^*G its cotangent bundle and by $\Pi : T^*G \to G$ the canonical projection. Let X_i $(i \leqslant n)$ be a basis of the Lie algebra $\mathfrak{g}$ of G and let $\widetilde{X}_i$ be the corresponding left invariant vector fields on G. If θ^i are the left invariant 1-forms on G such that $\theta^i(\widetilde{X}_j) = \delta^i_j$ and if $p_i : T^*G \to \mathbb{R} : \xi \to \xi(\widetilde{X}_i)$ one checks that the 1-forms $(\mathrm{d}p_i, \Pi^*\theta^i)$ form a basis of 1-forms on T^*G. The dual basis of vector fields (Z^i, Y_i) is such that

$$\Pi_* Z^i = 0 \qquad \Pi_* Y_i = \widetilde{X}_i.$$

The action of $G \times G$ onto G given by $(g, h) \cdot x = gxh^{-1}$ $(g, h, x \in G)$ lifts to T^*G; this action is hamiltonian. The vector fields corresponding to the left action have for value at ξ $(\in T^*G)$ $\mathrm{Ad}\,\Pi(\xi)^{-1} \cdot Y_i(\xi)$, the vector fields associated to the right action are $Y_i(\xi) + c_{ij}{}^k p_k(\xi) Z^j(\xi)$ ($c_{ij}{}^k$ = structure constants of $\mathfrak{g}$ in the basis X_i) and the corresponding functions are precisely the p_i's.

The linear injective map $\mathfrak{g} \to N : X_i \to p_i$ extends to an injective map $\varphi^{-1} : \mathfrak{U}(\mathfrak{g})$ (= universal envelopping algebra of $\mathfrak{g}$) $\to N : \langle X_{i_1} \ldots X_{i_k}\rangle \underset{\text{def}}{=} \frac{1}{k!} \sum_{\sigma \in S_k} X_{i_{\sigma(1)}} \circ \ldots \circ X_{i_{\sigma(k)}} \to p_{i_1} \ldots p_{i_k}$, whose image is the set of polynomials in the p_i's with constant coefficients.

THEOREM [5]. *On the cotangent bundle T^*G of an arbitrary Lie group G there exist a $*$ product having the following properties*

(i) *for all $f \in C^\infty(G)$, for all $u \in C^\infty(T^*G)$ one has*

$$\Pi^*f * u = \Pi^*f \cdot u + \sum_{r=1}^{\infty} (-1)^r \frac{\nu^r}{r!} \Pi^*(\widetilde{X}_{i_1} \ldots \widetilde{X}_{i_r} f)(Z^{i_1} \ldots Z^{i_r} u)$$

(ii) *for all P, Q monomials of degree k, k' in the p_i's one has*

$$P * Q = \sum_{r=0}^{k+k'-1} (2\nu)^r \varphi^{-1}(\varphi(P) \cdot \varphi(Q))_{k+k'-r}.$$

For an element $a \in \mathfrak{U}(\mathfrak{g})$, one denotes by a_ℓ the projection of a on the subspace $\mathfrak{U}^\ell(\mathfrak{g}) = \varphi$ (homogeneous polynomials of degree ℓ) parallely to the subspace

$$\bigoplus_{\substack{r=0\\ r\neq \ell}}^{\infty} \mathfrak{U}^r(\mathfrak{g})$$

(iii) *in particular when* $P = p_i$:

$$p_i * Q = \sum_{r=0}^{k'} \frac{(-2\nu)^r}{r!} B_r p_{j_r} c_{ik_1}^{j_1} c_{j_1 k_2}^{j_2} \dots c_{j_{r-1}k_r}^{j_r} (Z^{k_1} \dots Z^{k_r} Q)$$

where B_r *is the r-th Bernouilli number.*

(iv) *the* $*$ *product is entirely determined by properties* (i) *and* (iii).

PROPOSITION 1. *The* $*$ *product on* T^*G *defined by the preceding theorem is strongly invariant by* $G \times G$.

Proof. The geometrical invariance by the lift of the left action of G on G is a consequence of the following remarks:

(a) $(L^*_{g^{-1}})^* \Pi^* f = \Pi^* L^*_g f \qquad \forall g \in G$

(b) $L^*_g(\widetilde{X}_i f) = \widetilde{X}_i(L^*_g f) \qquad \forall g \in G, \quad \forall i = 1 \dots n$

(c) $(L^*_{g^{-1}})^*(Z^i u) = Z^i((L^*_{g^{-1}})^* u) \qquad \forall g \in G, \quad \forall i = 1 \dots n$

(d) $(L^*_{g^{-1}})^* p_j = p_j \qquad \forall g \in G, \quad \forall j = 1 \dots n.$

From these remarks we deduce the geometrical invariance of $u * v$ when either $u = \Pi^* f$ and v is arbitrary, either u and v are polynomials in the p_i's with constant coefficients. To prove geometrical invariance for arbitrary u and v in N, it is enough, as the $*$ product is defined by bidifferential operators, to prove it when u and v are polynomials in p_i's with coefficients which are functions on G; this last point is achieved by a recurrence argument on the degree of the polynomials in p_i's.

Similarly geometrical invariance by the lift of the right action of G on G results from a few simple observations

(a') $(R^*_g)^* \Pi^* f = \Pi^* R^*_{g^{-1}} f \qquad \forall g \in G$

(b') $R^*_{g^{-1}} \widetilde{X}_i f = (\mathrm{Ad}\, g^{-1})^k_i \widetilde{X}_k (R^*_{g^{-1}} f) \qquad \forall g \in G, \quad \forall i = 1 \dots n$

(c') $(R^*_g)^* Z^i u = (\mathrm{Ad}\, g)^i_k Z^k ((R^*_g)^* u) \qquad \forall g \in G, \quad \forall i = 1 \dots n$

(d') $(R^*_g)^* p_j = (\mathrm{Ad}\, g^{-1})^\ell_j p_\ell \qquad \forall g \in G, \quad \forall j = 1 \dots n.$

A recurrence argument similar to the one sketched above proves the invariance of the $*$ product.

To get the strong invariance by the lift of the left action of G one observes that formula (iii) of the theorem gives:

$$\frac{1}{2\nu}(p_i * p_j - p_j * p_i) = \{p_i, p_j\}.$$

For the strong invariance by the lift of the right action of G one remarks that the function associated to the element X_i of $\mathfrak{g}$ is $(\mathrm{Ad}\, x^{-1})_i^k p_k$ and uses the geometrical invariance of the $*$ product.

PROPOSITION 2. *The two geometrically invariant $*$ products on T^*S^3, constructed so far are distinct and invariantly equivalent.*

Proof. To show that they are distinct we observe that

$$p_i * p_j = p_i p_j + \nu\{p_i p_j\} + 4\nu^2 \delta_{ij} \qquad \text{(Moyal)}$$

$$p_i * p_j = p_i p_j + \nu\{p_i p_j\} \qquad \text{(intrinsic)}.$$

To prove that they are invariantly equivalent, we remark that $0 = H^2_{\text{de Rham}}(T^*S^3) = H^2_{\text{de Rham , inv by so(4)}}(T^*S^3)$ and that there exists an $so(4)$ invariant torsion free connection on T^*S_3 [9].

4. SPECTRUM OF THE HYDROGEN ATOM

We first compute the spectrum of the hamiltonian H using Moyal $*$ product on T^*S^3 and the corresponding Weyl transform. Recall that

$$H = -\frac{1}{2P^2}$$

and that one has:

$$\sum_{i=1}^{3} p_i^2 = h^2 + L^2 = P^2$$

so that

$$P^2 = \sum_{i=1}^{3} p_i * p_i - 12\nu^2.$$

When using the Weyl transform, it will be easier to deal with a $*$ polynomial in the p_i's than to a rational function. We thus compute

$$\begin{aligned}P^2 * F(P^2) - F(P^2) * P^2 &= \sum_i (p_i * p_i * F - F * p_i * p_i)\\ &= \sum_i [p_i * (p_i * F - F * p_i) + (p_i * F - F * p_i) * p_i]\\ &= 2\nu \sum_i (p_i * \{p_i, F\} + \{p_i, F\} * p_i)\end{aligned}$$

as p_i is a polynomial of degree 2 on ω. Now

$$\{p_i, F\} = F'\{p_i, P^2\} = 0$$

and thus $P^2 * F(P^2)$ is a formal series containing only even terms and truncated at order 4 as P^2 is a polynomial of degree 4 on ω. Hence

$$P^2 * F(P^2) = P^2 \cdot F(P^2) + \frac{\nu^2}{2!} \mathfrak{P}_2(P^2, F) + \frac{\nu^4}{4!} \mathfrak{P}_4(P^2, F).$$

The invariance by $so(4)$ implies that each of the term is a function of P^2 only. A direct computation shows that:

$$\mathfrak{P}_2(P^2, F) = 16P^2(3F' + P^2F'')$$

$$\mathfrak{P}_4(P^2, F) = 96(18F' + 57P^2F'' + 32P^4F''' + 4P^6F^{\mathrm{iv}}).$$

Hence when $F = \dfrac{1}{P^2}$ one gets

$$\mathfrak{P}_2\left(P^2, \frac{1}{P^2}\right) = -\frac{16}{P^2} \qquad \mathfrak{P}_4\left(P^2, \frac{1}{P^2}\right) = 0.$$

This implies that

$$H * \frac{1}{H} = 1 + 16\nu^2 H.$$

Schrödinger equation reads:

$$\psi * H = E\psi$$

which by virtue of the previous relation is equivalent to:

$$\psi * \frac{1}{H} = \frac{1 + 16\nu^2 E}{E} \psi$$

or also to:

$$(\sum_i p_i * p_i) = \frac{1 - 8\nu^2 E}{-2E} \psi.$$

DEFINITION. *The* Weyl transform W *on* T^*S^3, *associated to the Moyal product, is the homomorphism of the algebra* $(A, *)$ $(A = \{$*polynomials in the* p_i*'s with coefficients which are smooth functions on* $S^3\})$ *into the algebra* $(\mathbf{A}, 0)$ $(\mathbf{A} =$ *algebra of self-adjoint operators on* $L^2(S^3))$ *which is such that:*

(i) $W(p_i) = 2\nu \widetilde{X}_i$

(ii) $W(\Pi^* g) = g \cdot \mathrm{Id}$ $\qquad (g : S^3 \to \mathbb{R};\ \Pi : T^*S^3 \to S^3)$

(iii) $W(f * g) = W(f) \circ W(g)$.

As in the flat $(\mathbb{R}^{2n})$ case we interpret ψ as the linear map associated to an analytic function φ on S^3 by

$$\langle \psi, f\rangle = (W(f)\varphi)(e) \qquad (e = \textit{unit of } SU(2)).$$

Schrödinger equation now implies that:

$$4\nu^2 \Delta\varphi = \frac{1 - 8\nu^2 E}{-2E}\ \varphi$$

where Δ is the Laplace Beltrami operator on S^3. This gives the spectrum as

$$\frac{1 - 8\nu^2 E}{-2E} = -4\nu^2(n+2)n$$

or:

$$E = \frac{1}{8\nu^2(n+1)^2}\ .$$

When $\nu = \dfrac{i\hbar}{2}$ one has the usual spectrum of the hydrogen atom [1].

Computation of the spectrum of H with the intrinsic $*$ product and the corresponding Weyl transform starts in the same way. One has

$$H = -\frac{1}{2P^2} \qquad\qquad P^2 = \sum_i p_i^2 = \sum_i p_i * p_i.$$

As above:

$$P^2 * F(P^2) = F(P^2) * P^2$$

and thus $P^2 * F(P^2)$ is a formal series containing only even terms. The invariance by $so(4)$ implies that each term is a function of P^2 alone. But the series is not truncated at order 4. Furthermore a brutal calculation shows that the first term has a coefficient which is totally different from the one appearing in the Moyal product:

$$H * \frac{1}{H} = 1 - \frac{32\nu^2}{3} H + \dots .$$

This is already an indication that the spectrum will be different. We shall now prove that the spectra are indeed different, in a sequence of short lemmas.

LEMMA 1. *Let g be a smooth function of P^2. Then*

$$P^2 * g = P^2 \cdot g + \sum_{t>0} \nu^{2t} \left[\sum_{r>0}^{2t} a_r^t g^{r/} (P^2)^{1+r-t} \right]$$

where a_r^t is a real number and $g^{r/}$ is the r^{th} derivative of g.

This is proved using formula (iii) of the theorem of §3, and the fact that by invariance each term is a function of P^2 above.

LEMMA 2. *Let f, g be smooth functions of P^2. Then*

$$f * g = fg + \sum_{t>0} \nu^{2t} \left[\sum_{i,j>0}^{2t} a_{ij}^t f^{i/} g^{j/} (P^2)^{i+j-t} \right]$$

where a_{ij}^t is a real number.

To prove this lemma one first observes that it is enough to prove it when f is a polynomial as the $*$ product is given by differential operators. One then proceeds by recurrence on the degree of f.

This implies that:

$$P^2 * \frac{1}{P^2} = 1 + \sum_{t>0} \nu^{2t} a_t^n \frac{1}{(P^2)^t} .$$

LEMMA 3. *The following formal identity holds*

$$\left(* \frac{1}{P^2} \right)^t \underset{\text{def}}{=} \frac{1}{P^2} * \dots * \frac{1}{P^2} = \frac{1}{(P^2)^t} + \sum_{s>0} \nu^{2s} c_t^s \frac{1}{(P^2)^{t+s}}$$

where c_t^s is a real number.

This is proved by induction on t.

Using lemma 3 one sees that there exist real numbers a_t such that

$$\frac{1}{P^2} * P^2 = 1 + \sum_{t>0} \nu^{2t} a_t \left(\frac{1}{P^2} * \ldots * \frac{1}{P^2} \right) \qquad (t \text{ times})$$

Going back to Schrödinger's equation we get:

$$\psi * H * \frac{1}{H} = \psi \quad (1 + \sum_{t>0} \nu^{2t} a_t'(H * \ldots * H))$$

$$= \psi(1 + \sum_{t>0} \nu^{2t} a_t' E^t) = E\psi * \frac{1}{H}$$

or equivalently that $(1 + \sum_{t>0} \nu^{2t} a_t' E^t)\, \frac{1}{E}$ is an eigenvalue of $\frac{1}{H}$. Using the Weyl transform associated to this product we see as above that there exist an integer m such that:

$$\frac{1}{E}(1 + \sum_{t>0} \nu^{2t} a_t' E^t) = 8\nu^2 m(m+2).$$

Assume that the spectrum of H coincides with the one obtained with the Moyal $*$ product. Then for any integer n, there would exist a integer m such that

$$(n+1)^2 \left(1 + \sum_{t>0} \frac{a_t''}{(n+1)^{2t}} \right) = m(m+2).$$

This is easily shown to be impossible and thus the spectrum of H is not the one given by the Moyal $*$ product. One can prove a slightly stronger result, namely that the spectrum is not the form:

$$E = \frac{1}{8\nu^2(n+1)^2} + K \qquad (K \geqslant 0).$$

We are for the moment unable to compute the spectrum of H.

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