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LETTER TO THE EDITOR

On the canonical equivalence of the Kepler problem in coordinate and momentum spaces

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Abstract. It is shown that the dynamics of the hydrogen atom in elliptic cylindrical coordinates on the Fock hypersphere S^3 in momentum space is canonically equivalent to the R^3 (usual position space) dynamics. The implication to the semiclassical quantisation procedure of the hydrogen atom in a weak magnetic field is briefly discussed.

Even though the quantum dynamics of a hydrogen atom in a uniform magnetic field associated with the quadratic Zeeman interaction, $H_Q=\frac{1}{8}B^2(x^2+y^2)$, is non-separable, the O(4) symmetry of the hydrogen atom may be used to obtain an exact separation of the Schrödinger equation represented on the Fock hypersphere S^3 in momentum space in the weak-field limit, as noted recently by Herrick (1982). On the other hand, it is being increasingly realised that an alternative route to the analysis of the problem is to treat it as a nonlinear dynamical system and then perform a semiclassical quantisation (Gutzwiller 1977, Solovev 1982, Robnik 1982, Reinhardt and Farrelly 1982, Delos *et al* 1983). From this point of view, the classical dynamics in the associated momentum space is of fundamental interest for an understanding of the quantal problem. Accordingly it becomes necessary to establish that the transformations between R^3 and S^3 are canonical so that conjugate pairs may be defined on S^3. In this letter we point out that the elliptic cylindrical coordinate parametrisation of the Fock sphere S^3 employed by Herrick provides an exact canonical transformation of the R^3 dynamics in the field free case ($B=0$). We also note how this parametrisation can be extended to include the magnetic field so that at least in the situation $B\to 0$, Solovev's procedure of semiclassical quantisation (Solovev 1982) can be improved.

Let us consider the pure Kepler Hamiltonian (without an external field):

$$H=\tfrac{1}{2}\boldsymbol{v}^2-r^{-1} \tag{1}$$

where $\boldsymbol{v}$ $(=\boldsymbol{p})$ are the canonical conjugate momenta to $\boldsymbol{r}=(x,y,z)\equiv(x_1,x_2,x_3)\in R^3$. We have chosen the units such that charge and mass are unity. Then, the equation of motion is

$$\dot{\boldsymbol{r}}=\boldsymbol{v} \qquad \dot{\boldsymbol{v}}=-\boldsymbol{r}/r^3. \tag{2}$$

We define the Fock sphere S^3 (Bander and Itzykson 1966) specified by the coordinates

$$\boldsymbol{u}=(r/n)\boldsymbol{v} \qquad u_4=(n^2\boldsymbol{v}^2-1)/(n^2\boldsymbol{v}^2+1)=(1-r/n^2) \tag{3}$$

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where

$$n \equiv (-2E)^{-1/2}, \tag{4}$$

E being the energy of the hydrogen atom which is negative throughout the present discussion. The four-vector $\mathrm{u} \equiv (\boldsymbol{u}, u^4)$, then lies in the unit sphere S^3:

$$\mathrm{u}^2 = \boldsymbol{u}^2 + u_4^2 = 1. \tag{5}$$

If we now consider the associated angular momentum vector $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{v}$ and the normalised Lenz vector $\boldsymbol{K} = n\{\boldsymbol{v} \times (\boldsymbol{r} \times \boldsymbol{v}) - \boldsymbol{r}/r\}$ $(= (-2E)^{-1/2}\boldsymbol{A})$, we can express them in terms of the four-vector u and its time derivative $\dot{\mathrm{u}}$ as

$$\boldsymbol{L} = n^4(1-u_4)(\boldsymbol{u} \times \dot{\boldsymbol{u}}) \tag{6a}$$

$$\boldsymbol{K} = n^4(1-u_4)(\boldsymbol{u}\dot{u}_4 - u_4\dot{\boldsymbol{u}}) \tag{6b}$$

which satisfy the basic identity (the so-called Casimir identity)

$$\boldsymbol{L}^2 + \boldsymbol{K}^2 = n^2. \tag{7}$$

On the other hand, it is known (Kalnins *et al* 1976) that the quantised versions of $\boldsymbol{L}$ and $\boldsymbol{K}$ corresponding to the O(4) group of the hydrogen atom satisfy the Lie algebra LO(4):

$$[L_i, L_j] = \mathrm{i}\varepsilon_{ijk}L_k \qquad [L_i, K_j] = \mathrm{i}\varepsilon_{ijk}K_k \qquad [K_i, K_j] = \mathrm{i}\varepsilon_{ijk}L_k \qquad (i, j, k = 1, 2, 3),$$

which is defined in terms of vector spaces of functions on R^3 as well as on S^3. On R^3 they have the usual expressions:

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p} \qquad \boldsymbol{K} = (-2E)^{-1/2}[\tfrac{1}{2}(\boldsymbol{p} \times \boldsymbol{L} - \boldsymbol{L} \times \boldsymbol{p}) - \boldsymbol{r}/r] \tag{8}$$

with $\boldsymbol{r} = (x, y, z)$, $\boldsymbol{p} = -\mathrm{i}(\partial_x, \partial_y, \partial_x)$, while on S^3 they have the form (Kalnins *et al* 1976)

$$\boldsymbol{L} = \boldsymbol{u} \times \boldsymbol{p}_u \qquad \boldsymbol{K} = \boldsymbol{u}p_{u_4} - u_4\boldsymbol{p}_u \tag{9}$$

with $\boldsymbol{p}_u = -\mathrm{i}\partial_{\boldsymbol{u}}$, $p_{u_4} = -\mathrm{i}\partial_{u_4}$.

Thus, in the related classical problem the commutators for (8) and (9) will be replaced by the Poisson brackets and the linear operators $\boldsymbol{L}$ and $\boldsymbol{K}$ become the associated classical vectors in R^3 and also in S^3. A comparison of the expressions ($6a$, b) with (9) yields the relations between $\dot{\mathrm{u}}$ and p_u as follows

$$\dot{\boldsymbol{u}} = [n^4(1-u_4)]^{-1}\boldsymbol{p}_u \qquad \dot{u}_4 = [n^4(1-u_4)]^{-1}p_{u_4}. \tag{10a}$$

This set of relations is combined with another set, to be derived from the equations of motion (2), i.e.

$$\dot{\boldsymbol{p}}_u = -[n^2(1-u_4)]^{-1}\boldsymbol{u} \qquad \dot{p}_{u_4} = -[n^2(1-u_4)]^{-1}u_4, \tag{10b}$$

which may be regarded as the equations of the Kepler motion in S^3.

At this stage, however, we note the important fact that the above set of equations of motion cannot be canonical equations of motion because of the presence of the factor $n^{-4}(1-u_4)^{-1}$ on the right-hand sides of each member of equations ($10a$, b). In other words the presence of this factor precludes the canonicity of the variables $(\boldsymbol{u}, u_4)$ and $(\boldsymbol{p}_u, p_4)$. In fact, without this extra factor this dynamics may be shown to be equivalent to that of a free particle on a 3-sphere (Lakshmanan and Eswaran 1975, Higgs 1979) which can be derived from a suitable Hamiltonian. The reason for this inconvenience is essentially that the four-vector u and its 'conjugate' momenta p_u are redundant variables for S^3-dynamics. Therefore, we desire some other set of variables that is exactly a canonical set on S^3, equivalent to the original space R^3†. Here, we show that the elliptic cylindrical coordinates fulfil this requirement.

The system of elliptic cylindrical coordinates of type I (Kalnins *et al* 1976, Herrick 1982) is defined by

$$u_1 = \mathrm{sn}\,\alpha\,\mathrm{dn}\,\beta\cos\phi \qquad u_2 = \mathrm{sn}\,\alpha\,\mathrm{dn}\,\beta\sin\phi \tag{11a, b}$$

$$u_3 = \mathrm{dn}\,\alpha\,\mathrm{sn}\,\beta \qquad u_4 = \mathrm{cn}\,\alpha\,\mathrm{cn}\,\beta \tag{11c, d}$$

where $\mathrm{sn}\,\alpha = \mathrm{sn}(\alpha, k)$, $\mathrm{sn}\,\beta = \mathrm{sn}(\beta, k')$ etc are the Jacobian elliptic functions, k and $k' = (1-k^2)^{1/2}$ being the modulus and complementary modulus, respectively. From the identity $\mathrm{sn}^2\,\alpha\,\mathrm{dn}^2\,\beta + \mathrm{dn}^2\,\alpha\,\mathrm{sn}^2\,\beta + \mathrm{cn}^2\,\alpha\,\mathrm{cn}^2\,\beta = 1$, it is easy to see that the unit sphere (5) is parametrised by these coordinates α, β, ϕ and their respective momenta p_α, p_β, p_ϕ defined by

$$\begin{aligned} p_{\alpha,\beta} &= n^2 r(k^2\,\mathrm{cn}^2\,\alpha + k'^2\,\mathrm{cn}^2\,\beta)(\dot\alpha, \text{ or } \dot\beta), \\ p_\phi &= n^2 r\,\mathrm{sn}^2\,\alpha\,\mathrm{dn}^2\,\beta\dot\phi. \end{aligned} \tag{11e}$$

Thus, what we want to prove is that the transformation from the Cartesian coordinates in the position space and their momenta $\{x, y, z; p_x, p_y, p_z\} \in R^3 \times R^3$ to the set $\{\alpha, \beta, \phi; p_\alpha, p_\beta, p_\phi\} \in S^3 \times R^3$ is indeed a canonical transformation. This is true, iff the canonical Poisson bracket on $R^3 \times R^3$ is preserved in $S^3 \times R^3$ to within a non-zero constant factor (Saletan and Cramer 1971).

The proof of our assertion proceeds as follows. We consider the set of fifteen Poisson brackets

$$\{x_i, x_j\} = \{p_i, p_j\} = 0 \qquad \{x_i, p_j\} = \delta_{ij} \qquad (i, j = 1, 2, 3) \tag{12}$$

and define the Poisson bracket for X and Y by $\{X, Y\} = \Sigma_{i=1}^{3}((\partial X/\partial x_i)\partial Y/\partial p_i - (\partial X/\partial p_i)\partial Y/\partial x_i)$; we then calculate the other set of fifteen Poisson brackets among $\{\alpha, \beta, \phi; p_\alpha, p_\beta, p_\phi\}$ to show that the latter is really a canonical set. However, this is equivalent to showing the converse that under the assumption of the fifteen canonical commutation relations

$$\begin{aligned} \{\alpha, \beta\} &= \{\alpha, \phi\} = \{\beta, \phi\} = \{p_\alpha, p_\beta\} = \{p_\alpha, p_\phi\} = \{p_\beta, p_\phi\} \\ &= \{\alpha, p_\beta\} = \{\beta, p_\alpha\} = \{\phi, p_\alpha\} = \{\phi, p_\beta\} = \{\alpha, p_\phi\} = \{\beta, p_\phi\} = 0 \\ &\quad \{\alpha, p_\alpha\} = \{\beta, p_\beta\} = \{\phi, p_\phi\} = 1, \end{aligned} \tag{13}$$

the former relations (12) hold, where now the Poisson bracket is defined by $\{X, Y\} = (\partial X/\partial\alpha)\partial Y/\partial p_\alpha - (\partial X/\partial p_\alpha)\partial Y/\partial\alpha + (\text{the } \beta \text{ term}) + (\text{the } \phi \text{ term})$. We adopt the latter procedure, since it is possible to express the former set as functions of the latter: We have

$$p_i = [n(1-u_4)]^{-1}u_i \qquad x_i = -n[(1-u_4)p_{u_i} + p_{u_4}u_i] \qquad (i = 1, 2, 3) \tag{14}$$

and the elliptic-cylindrical parametrisation (11a–e) provides the expressions of u_i and

† With regard to this redundant structure in (10a, b), it may be of further interest to note that the second members of these equations, i.e. $\dot u_4$ and $\dot p_{u4}$, are closed by themselves, and thus can be reduced to a second-order differential equation for the radius r (note r is related to u_4 as indicated in (3)) and is equivalent to the well known Kepler equations: $r = n^2(1 - e\cos\psi)$, $t = n^3(\psi - e\sin\psi)$, where ψ is the eccentric anomaly. Thus, once $r(t)$ is determined, the extra factor $n^4(1-u_4)$ becomes a known function of time and may be absorbed into the time variable in (10a, b).

p_{u_i}, $i = 1, 2, 3$ and 4, in terms of α, β, ϕ and p_α, p_β, p_ϕ. Thus

$$p_x = \frac{\operatorname{sn}\alpha \operatorname{dn}\beta}{n(1-\operatorname{cn}\alpha \operatorname{cn}\beta)}\cos\phi \qquad p_y = \frac{\operatorname{sn}\alpha \operatorname{dn}\beta}{n(1-\operatorname{cn}\alpha \operatorname{cn}\beta)}\sin\phi \tag{15a}$$

$$p_z = \frac{\operatorname{dn}\alpha \operatorname{sn}\beta}{n(1-\operatorname{cn}\alpha \operatorname{cn}\beta)}; \tag{15b}$$

$$x = n\{-\operatorname{dn}\alpha \operatorname{dn}\beta(\operatorname{cn}\alpha - \operatorname{cn}\beta)p_\alpha/J + \operatorname{sn}\alpha \operatorname{cn}\beta(k^2 \operatorname{cn}\alpha + k'^2 \operatorname{cn}\beta)p_\beta/J\}\cos\phi$$

$$+ n\frac{1-\operatorname{cn}\alpha \operatorname{cn}\beta}{\operatorname{sn}\alpha \operatorname{dn}\beta}p_\phi \sin\phi \tag{15c}$$

$$y = n\{\text{same as above}\}\sin\phi - n\frac{1-\operatorname{cn}\alpha \operatorname{cn}\beta}{\operatorname{sn}\alpha \operatorname{dn}\beta}p_\phi \cos\phi \tag{15d}$$

$$z = n\{\operatorname{sn}\alpha \operatorname{cn}\beta(k^2 \operatorname{cn}\alpha + k'^2 \operatorname{cn}\beta)p_\alpha/J + \operatorname{dn}\alpha \operatorname{dn}\beta(\operatorname{cn}\alpha - \operatorname{cn}\beta)p_\beta/J\} \tag{15e}$$

where $J \equiv k^2 \operatorname{cn}^2\alpha + k'^2 \operatorname{cn}^2\beta$.

At first sight, it looks a formidable task to calculate the fifteen Poisson brackets for the above six expressions, but it turns out that there exists a keyword identity by which most brackets are simplified to show that these are in fact a set of canonical variables satisfying (12). This identity reads:

$$\operatorname{sn}^2\alpha \operatorname{sn}^2\beta(k^2 \operatorname{cn}\alpha + k'^2 \operatorname{cn}\beta)^2 + \operatorname{dn}^2\alpha \operatorname{dn}^2\beta(\operatorname{cn}\alpha - \operatorname{cn}\beta)^2$$

$$= (k^2 \operatorname{cn}^2\alpha + k'^2 \operatorname{cn}^2\beta)(1-\operatorname{cn}\alpha \operatorname{cn}\beta)^2 \tag{16}$$

which, with the aid of the Casimir identity (7), ensures the identity

$$x^2 + y^2 + z^2 = r^2 = n^4(1-u_4)^2. \tag{17}$$

Upon establishing, thus, the canonicity of the pair (α, β, ϕ) and $(p_\alpha, p_\beta, p_\phi)$, it is now possible to see the separability of the Kepler motion on S^3. First, we write down the Casimir identity (7) in terms of this canonical set so that

(I)
$$\frac{p_\alpha^2 + p_\beta^2}{k^2 \operatorname{cn}^2\alpha + k'^2 \operatorname{cn}^2\beta} + \frac{p_\phi^2}{\operatorname{sn}^2\alpha \operatorname{dn}^2\beta} = n^2. \tag{18}$$

Then, because of the cyclicity of the coordinate ϕ,

(II)
$$p_\phi (= n^4(1-\operatorname{cn}\alpha \operatorname{cn}\beta)\operatorname{sn}^2\alpha \operatorname{dn}^2\beta\dot\phi) = m \tag{19}$$

which is shown from ($15a$–d) to be equal to the z component of the angular momentum, $xp_y - yp_x$. This second integral of motion is combined with I to yield the third integral:

(III)
$$\frac{k'^2 \operatorname{cn}^2\beta p_\alpha^2 - k^2 \operatorname{cn}^2\alpha p_\beta^2}{k^2 \operatorname{cn}^2\alpha + k'^2 \operatorname{cn}^2\beta} + \frac{k'^2 p_\phi^2 \operatorname{cn}^2\alpha \operatorname{cn}^2\beta}{\operatorname{sn}^2\alpha \operatorname{dn}^2\beta} = \lambda \tag{20}$$

where the left-hand side is shown to be a hyperbolic form of the Lenz vector, namely a generalisation of Solovev (1982):

$$(1-k^2)(K_x^2 + K_y^2) - k^2 K_z^2 = k^2 n^2 \Lambda \tag{21}$$

so that

$$\lambda = k^2 n^2 \Lambda. \tag{21a}$$

From these, the desired separation is given by

$$p_\alpha^2 = b - k^2 n^2 \,\mathrm{sn}^2\,\alpha - m^2/\mathrm{sn}^2\alpha \tag{22a}$$

$$p_\beta^2 = -b + n^2 \,\mathrm{dn}^2\,\beta + k^2 m^2/\mathrm{dn}^2\beta \tag{22b}$$

where

$$b = k^2 n^2 (1+\Lambda) + m^2. \tag{22c}$$

The two action integrals for the α and β coordinates in (22), i.e.

$$J_\alpha = \frac{1}{\pi}\int_0^{2K} p_\alpha \,\mathrm{d}\alpha \qquad J_\beta = \frac{1}{\pi}\int_0^{2K'} p_\beta \,\mathrm{d}\beta \tag{23}$$

where K and K' are the complete elliptic integrals of the first kind associated with $\mathrm{sn}(\alpha, k)$ and $\mathrm{sn}(\beta, k')$, respectively, will provide the semiclassical quantisation of the two types of Kepler motion corresponding to a rotation and a libration of the Lenz vector. But, both can be unified in a complex plane such that

$$J_{\alpha,\beta} = \frac{1}{2\pi \mathrm{i}}\int_{C_{\alpha,\beta}} (-b + k^2 n^2 \,\mathrm{sn}^2\,\zeta + m^2/\mathrm{sn}^2\zeta)^{1/2}\,\mathrm{d}\zeta \tag{24}$$

where C_α and C_β are two intervals of the fundamental period along the real and imaginary axes of ζ; $0 \leqslant \mathrm{Re}\,\zeta < 4K$ and $0 \leqslant \mathrm{Im}\,\zeta < 4K'$, for any Jacobian elliptic function of a complex variable. Without an external field, the quantisation must yield the energy value $E = -\frac{1}{2}n^{-2}$, $n = 1, 2, \ldots$, irrespective of the separation parameter b in (24), which is assured from a more detailed examination of the integration (24).

An implication of the existence of the above two action integrals (24) is that, when a uniform magnetic field B is applied to the Kepler motion of a charged particle, a separation of the motion comes out in phase space in the limit $B \to 0$. This may be looked upon as a natural unperturbed motion of two degrees of freedom with a generally irrational winding number (Lichtenberg and Lieberman 1983) that will yield a KAM torus remaining undestroyed, when the perturbation strength B is increased to an extent.

The fact that the elliptic cylindrical parametrisation on the Fock sphere is a legitimate canonical set of variables equivalent to the R^3 dynamics should provide, in principle, a way to describe the diamagnetic Kepler motion with an arbitrary strength of B in terms of the set $\{\alpha, \beta, \phi; p_\alpha, p_\beta, p_\phi\}$. Under such circumstances, we can show that the Casimir identity I holds exactly if p_ϕ is replaced by $p_\phi + B$-term (involving α, β, p_α, p_β). However, the separability by means of III is no longer valid. Nevertheless, an extended formulation can be used to describe probable KAM tori by this analytic means, where the modulus k is unrestricted to the value obtained by Solovev (Hasegawa *et al* 1984).

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