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On an Analyticity Property in (Complex) Phase Space

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Abstract

Some consequences of one-valuedness on the real phase space for certain analytic functions over the complex phase space of a Hamiltonian system are demonstrated. The Bohr–Sommerfeld quantisation conditions are reformulated as one-valuedness conditions for these functions on the complex phase space.

1. *Review of the Hamilton–Jacobi Theory and Action-Angle Variables*

The Hamilton equations of motion for a dynamical system

$$\frac{\partial H}{\partial p_i} = \dot{q}_i, \qquad \frac{\partial H}{\partial q_i} = -\dot{p}_i, \qquad i = 1, \ldots, n \tag{1.1}$$

can be transformed (in principle at least) via a canonical transformation to a set of dynamical variables (q_i', p_i') in terms of which the new Hamiltonian H' is identically zero. The transformed variables are then constants of the motion which may, for example, be taken as the $2n$ values of the old variables at some fixed time. The transformation thus provides a solution of the initial value problem for the system of equations (1.1).

Assuming the generating function $S(q, p', t)$ of the canonical transformation to be a function of the old coordinates, the new momenta and time, we have

$$H(q, p, t) + \frac{\partial S}{\partial t}(q, p', t) = H'(q', p', t) \equiv 0 \tag{1.2}$$

$$p_i = \frac{\partial S}{\partial q_i} \tag{1.3}$$

$$q_i' = \frac{\partial S}{\partial p_i'} \tag{1.4}$$

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Substituting the expression for p_i given by equation (1.3) into equation (1.2), one gets the Hamilton–Jacobi equation for S (Hamilton's principal function)

$$H\left(q, \frac{\partial S}{\partial q}, t\right) + \frac{\partial S}{\partial t} = 0 \tag{1.5}$$

The transformed momenta p', which are constants of the motion, may now be identified with the n non-trivial constants of integration c_i appearing in the solution of equation (1.5). Notice that one of the $n + 1$ constants of integration is trivial in the sense that it is purely additive and, therefore, the dynamical variables do not depend on it. When H contains no explicit time dependence one may separate S into a time-independent and a q-independent part, i.e.

$$S(q_i, c_i, t) = W(q_i, c_i) - Et \tag{1.6}$$

where

$$H\left(q_i, \frac{\partial W}{\partial q_i}\right) = E = H(p') \tag{1.7}$$

E is a constant which may be taken as c_1 and expressed as a function of the new momenta p' (constant by construction). The canonical transformation generated by W leaves H invariant. Notice that

$$\dot{q}_i' = \frac{\partial H}{\partial p_i'} = \nu_i$$

$$\dot{p}_i' = -\frac{\partial H}{\partial q_i'} = 0$$

so that

$$\begin{aligned} q_i' &= \nu_i t + \alpha_i \\ p_i' &= \beta_i \end{aligned} \tag{1.8}$$

So far we have not specified the constants except that one of them has been identified rather arbitrarily with the energy E. If one is dealing with vibration or rotation coordinates q_i of a separable system† one introduces new constants J_i as functions of the old c_i in the following way:

$$J_i = \oint \frac{\partial W(q, c_1, \ldots, c_n)}{\partial q_i}\, dq_i \tag{1.9}$$

† The necessary and sufficient conditions of separability of the Hamilton–Jacobi equation have been given by Levi-Civita (1904). They are

$$\frac{\partial H}{\partial p_k}\frac{\partial H}{\partial p_s}\frac{\partial^2 H}{\partial q_k \partial q_s} - \frac{\partial H}{\partial p_k}\frac{\partial H}{\partial q_s}\frac{\partial^2 H}{\partial q_k \partial p_s} - \frac{\partial H}{\partial q_k}\frac{\partial H}{\partial p_s}\frac{\partial^2 H}{\partial p_k \partial q_s} + \frac{\partial H}{\partial q_k}\frac{\partial H}{\partial q_s}\frac{\partial^2 H}{\partial p_k \partial p_s} = 0$$

See also Max Jammer (1966).

where the integration is over a complete cycle of vibration or rotation. The constant momenta p_i' are now identified with the new constants J_i. The new coordinates θ_i (corresponding to J_i) are derived by expressing $W(q, c_1, \ldots, c_n)$ as $W(q, J_1, \ldots, J_n)$ through equation (1.9) which determines c_i as functions of J_i and partial differentiation

$$\theta_i = \frac{\partial W(q, J_1, \ldots, J_n)}{\partial J_i} \tag{1.10}$$

From equations (1.7) and (1.8)

$$E = H(J_i) \tag{1.11}$$

$$\dot{\theta}_i = \frac{\partial H}{\partial J_i} = \nu_i(J_1, \ldots, J_n) \tag{1.12}$$

θ_i have the interesting property that during a complete cycle of variation of the coordinate q_j the change in θ_i is δ_{ij}. Since

$$\begin{aligned} \Delta\theta_i &= \oint \frac{\partial \theta_i}{\partial q_j} dq_j = \oint \frac{\partial^2 W}{\partial q_j \partial J_i} dq_j \\ &= \frac{\partial}{\partial J_i} \oint p_j dq_j = \delta_{ij} \end{aligned} \tag{1.13}$$

Thus it follows from equations (1.12) and (1.13) that ν_i is the frequency associated with the periodic motion of q_i and one may write for the coordinate q_i the Fourier series

$$q_i = \sum_{n=-\infty}^{+\infty} a_n \exp(2\pi i n \nu_i) \qquad (q_i\text{: vibration coordinate})$$

$$q_i - \lambda_i = \sum_{n=-\infty}^{+\infty} a_n \exp(2\pi i n \nu_i) \qquad (q_i\text{: rotation coordinate with period } \lambda_i) \tag{1.14}$$

We are now in a position to present the results of our investigation.

2. *Conjecture and Corollaries*

Theorem (conjecture). Suppose $f(p, q)$ is an analytic function over the complex phase space containing no explicit time dependence such that

(i) It is one-valued over the real phase space

(ii) $$\frac{d}{dt} f(p, q) = 2\pi \nu i f(p, q) \tag{2.1}$$

Then

$$\nu = \sum_{i=1}^{n} n_i \nu_i$$

where n_i are integers and $\nu_i = \partial H/\partial J_i$. We have not been able to prove this theorem in spite of the intuitive feeling that it must be true. This will not deter us from studying some of its consequences and checking them for specific dynamical systems.

Definition. The modified Poisson bracket $\{H(p, q), A(p, q)\}_{PB(j)}$ is defined as follows. Express $H(p, q)$ in terms of the actions J_i as explained above, $H(p, q) = H(J_1, \ldots, J_n)$. In this expression for H regard J_i $(i \neq j)$ as ordinary numbers and write J_j as a function of p, q through the integrated form of the equations of motion. With this understanding in mind calculate the Poisson bracket of $H(p, q)$ with $f(p, q)$ in the usual way. In terms of this definition we may now state the corollary to the above theorem.

Corollary 1. Suppose $f(p, q)$ is an analytic function over the complex phase space with no explicit time dependence such that

(i) it is one-valued over the real phase space;
(ii) ϕ is a function of p, q through its dependence on the Hamiltonian H, i.e. $\phi(p, q) \equiv \phi(H(p, q))$;
(iii) $$\{\phi(H(p, q)), f(p, q)\}_{PB(j)} = if(p, q) \tag{2.2}$$

Then the function ϕ must be such that its derivative is given by

$$\phi'(H) = \frac{1}{2\pi\nu_j n}$$

where n is an integer and

$$\nu_j = \frac{\partial H}{\partial J_i}(J_1, \ldots, J_n) \tag{2.3}$$

This is a straightforward consequence of the theorem. We first notice that

$$\begin{aligned}\{\phi(H(p, q)), f(p, q)\}_{PB} &= \phi'(H)\{H(p, q), f(p, q)\}_{PB} \\ &= \phi'(H)\frac{d}{dt}f(p, q)\end{aligned} \tag{2.4}$$

Thus if $f(p, q)$ is one-valued over the real phase space satisfying the equation

$$\{\phi(H(p, q)), f(p, q)\}_{PB} = if(p, q)$$

we get from the above theorem

$$\frac{1}{\phi'(H)} = 2\pi \sum_{i=1}^{n} \nu_i n_i \tag{2.5}$$

If we now use the modified Poisson bracket defined above, the terms $i \neq j$ on the right-hand side of equation (2.5) drop out and the corollary follows.

Corollary 2. For a system with one degree of freedom, let $f(p, q)$ be an analytic function over the complex phase space with no explicit time dependence such that

(i) it is one-valued over the real phase space;
(ii) ϕ is a function of p, q through its dependence on the Hamiltonian H, i.e.

$$\phi(p, q) \equiv \phi(H(p, q))$$

(iii) $$\{\phi(H(p, q)), f(p, q)\}_{PB} = if(p, q)$$

Then

$$\phi(E) = \frac{1}{2\pi n} \oint p(E, q)\, dq + c$$

where n is an integer, c is an arbitrary constant, and $p(E, q)$ is the explicit form of the function p obtained by solving $H(p, q) = E$. This follows immediately from Corollary 1.

Since

$$\phi'(H) = \frac{1}{2\pi\nu n} = \frac{1}{2\pi n} \frac{dJ}{dH}$$

can now be integrated to give

$$\phi(H) = \frac{1}{2\pi n} J + c$$

$$J = \oint p(H, q)\, dq$$

In Sections 3 and 4 we shall check the validity of Corollary 2 for the non-linear oscillator and the relativistic oscillator. In Section 5 we study the hydrogen atom and verify Corollary 1.

3. *Non-Linear Oscillator*

As the first example illustrating Corollary 2 we shall take the non-linear oscillator described by the Hamiltonian

$$H = \tfrac{1}{2}(p^2 + \omega^2 q^2) + \tfrac{1}{4}\lambda q^4, \qquad \lambda > 0 \tag{3.1}$$

We must find the function $\phi(H)$ such that the associated annihilation function $f(p, q)$ satisfying the equation

$$\{\phi(H(p, q)), f(p, q)\}_{PB} = if(p, q) \tag{3.2}$$

is one-valued over the real phase space (no branch cuts).† Once this is ensured, it follows from the foregoing argument that

$$\phi = \phi_m(E) = \frac{1}{2\pi m} \oint p(E, q)\, dq + c, \qquad m \text{ integer} \tag{3.3}$$

Thus the Bohr–Sommerfeld quantisation condition for the system is equivalent to

$$\phi_1(E_n) = n\hbar + c, \qquad n \text{ integer} \tag{3.4}$$

To facilitate the determination of ϕ we write equation (3.2) as

$$\phi'(H)\left(\frac{\partial H}{\partial p}\frac{\partial f}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial f}{\partial p}\right) = if \tag{3.5a}$$

i.e.

$$\phi'(H)\left[p\frac{\partial f}{\partial q} - (\omega^2 q + \lambda q^3)\frac{\partial f}{\partial p}\right] = if \tag{3.5b}$$

Define

$$\xi = \tfrac{1}{2}(-p^2 + \omega^2 q^2) + \tfrac{1}{4}\lambda q^4 \tag{3.6}$$

Then equation (3.5b) may be rewritten as

$$\phi'(H)\left(\frac{\partial f}{\partial \xi}\right)_H = \frac{i}{2} f \frac{1}{\sqrt{(H-\xi)}} \frac{\sqrt{\lambda}}{\omega^3}\left[\left(1 + \frac{2\lambda}{\omega^4}(\xi + H)\right)^{1/2} - 1\right]^{-1/2} \times \left(1 + \frac{2\lambda}{\omega^4}(\xi + H)\right)^{-1/2} \tag{3.7}$$

Thus, on integration of (3.7) we have

$$\omega\phi'(H)\log f(\xi, H) = \frac{1}{2}\int \frac{1}{\sqrt{(\xi^2 - H^2)}}\, \psi\left[\frac{2\lambda}{\omega^4}(\xi + H)\right] d\xi + \text{arbitrary function of } H \tag{3.8}$$

where

$$\psi(x) = \frac{\sqrt{x}}{\sqrt{2}}(1+x)^{-1/2}[(1+x)^{-1/2} - 1]^{-1/2}$$

$$= 1 - \tfrac{3}{8}x + \tfrac{35}{128}x^2 - \tfrac{231}{1024}x^3 + \ldots \tag{3.9}$$

† When f is one-valued everywhere over the complex phase space and not just over the real phase space, then the Bohr–Sommerfeld quantisation is equivalent to the usual quantisation.

This series expansion for ψ is, however, unnecessary for the following argument. Only the formal existence of such a series is all that is needed. Now,

$$\psi\left[\frac{2\lambda}{\omega^4}(\xi+H)\right]=\psi\left(\frac{2\lambda}{\omega^4}H\right)+\frac{2\lambda}{\omega^4}\xi\psi'\left(\frac{2\lambda}{\omega^4}H\right)+\left(\frac{2\lambda}{\omega^4}\xi\right)^2\frac{1}{2!}\psi''\left(\frac{2\lambda}{\omega^4}H\right)+\ldots \tag{3.10}$$

so that on the right-hand side of (3.8) we have to deal with integrals of the form

$$I_n=\int\frac{\xi^n}{\sqrt{(\xi^2-H^2)}}\,d\xi$$

$$I_n=\frac{n-1}{n}H^2I_{n-2}+\frac{1}{n}\xi^{n-1}\sqrt{(\xi^2-H^2)}$$

$$I_0=\log\left(\frac{\xi+\sqrt{(\xi^2-H^2)}}{H}\right)$$

$$I_1=\sqrt{(\xi^2-H^2)} \tag{3.11}$$

Collecting the terms on the right-hand side of (3.8) with the factor

$$\log\left(\frac{\xi+\sqrt{(\xi^2-H^2)}}{H}\right)=I_0$$

arising from integrating the even terms $\xi^{2p}/\sqrt{(\xi^2-H^2)}$ in the expansion (3.10), we get

$$\int\frac{1}{\sqrt{(\xi^2-H^2)}}\psi\left[\frac{2\lambda}{\omega^4}(\xi+H)\right]d\xi$$

$$=\left[\psi\left(\frac{2\lambda}{\omega^4}H\right)+\left(\frac{2\lambda}{\omega^4}H\right)^2\frac{1}{2!}\frac{1}{2}\psi''\left(\frac{2\lambda}{\omega^4}H\right)+\left(\frac{2\lambda}{\omega^4}H\right)^4\left(\frac{1}{4!}\frac{3}{4}\frac{1}{2}\psi^{\mathrm{IV}}\left(\frac{2\lambda}{\omega^4}H\right)\right.\right.$$

$$\left.+\ldots\right]I_0+R \tag{3.12}$$

where R consists of the remaining terms not containing the multiplicative factor I_0. Notice that

$$e^{I_0}=\frac{\omega q\left(1+\dfrac{\lambda}{2\omega^2}q^2\right)^{1/2}+ip}{\omega q\left(1+\dfrac{\lambda}{2\omega^2}q^2\right)^{1/2}-ip} \tag{3.13}$$

Comparing equations (3.8) and (3.12) we observe that the one-valuedness of f (analytic) over the real phase space leads to the condition

$$m\omega\phi'(H) = \tfrac{1}{2}\left[\psi\left(\frac{2\lambda}{\omega^4}H\right) + \left(\frac{2\lambda}{\omega^4}H\right)^2 \frac{1}{2!}\tfrac{1}{2}\psi''\left(\frac{2\lambda}{\omega^4}H\right) + \left(\frac{2\lambda}{\omega^4}H\right)^4 \frac{1}{4!} \times \tfrac{3}{4}\tfrac{1}{2}\psi^{\mathrm{IV}}\left(\frac{2\lambda}{\omega^4}H\right) + \ldots\right], \qquad m \text{ integer} \tag{3.14}$$

Now the right-hand side of equation (3.14) can be expressed in a closed form, viz.

$$\text{Right-hand side of equation (3.14)} = \frac{1}{\pi}\int_0^{\pi/2}\left[\psi\left(\frac{2\lambda}{\omega^4}H\right) + \frac{1}{2!}\left(\frac{2\lambda}{\omega^4}H\right)^2 \times \cos^2\theta\,\psi''\left(\frac{2\lambda}{\omega^4}H\right) + \ldots\right] d\theta$$

$$= \frac{1}{\pi}\int_0^{\pi}\psi\left[\frac{2\lambda}{\omega^4}H(1+\cos\theta)\right] d\theta \tag{3.15}$$

so that

$$\phi_m'(E) = \frac{1}{\pi\omega m}\int_0^{\pi}\psi\left[\frac{2\lambda E}{\omega^4}(1+\cos\theta)\right] d\theta \tag{3.16}$$

Let

$$x = \frac{2\lambda E}{\omega^4}(1+\cos\theta), \qquad a = \frac{2\lambda E}{\omega^4}$$

$$\phi_m'(E) = \frac{1}{\pi\omega m}\int_0^{2a}\psi(x)x^{-1/2}(2a-x)^{-1/2}\,dx$$

$$= \frac{1}{\sqrt{(2)}\pi\omega m}\int_0^{2a}(1+x)^{-1/2}[(1+x)^{1/2}-1]^{-1/2}(2a-x)^{-1/2}\,dx$$

$$= \frac{1}{2\pi m}\oint\left(2E - \omega^2 q^2 - \frac{\lambda}{2}q^4\right)^{-1/2} dq \tag{3.17}$$

i.e.

$$\phi_m(E) = \frac{1}{2\pi m}\oint\left(2E - \omega^2 q^2 - \frac{\lambda}{2}q^4\right)^{1/2} dq + c$$

$$= \frac{1}{2\pi m}\oint p(E,q)\,dq + c \tag{3.18}$$

Thus we have shown explicitly that function $\phi(H)$ determined from the requirement of one-valuedness of $f(p, q)$ over the real phase space is indeed such that

$$m\phi(E_k) = k\hbar + c$$

is equivalent to the Bohr–Sommerfeld quantisation.

4. *Relativistic Oscillator*

We define the relativistic oscillator as a particle whose equation of motion is

$$m\ddot{x}_\mu + \omega^2\{(x_\mu - y_\mu) + (x \, . \, \dot{x} - y \, . \, \dot{x})\dot{x}_\mu\} = 0$$

$$\ddot{y}_\mu = 0 \tag{4.1}$$

where x_μ is the four-vector specifying the particle in space time, and y_μ is a four-vector which may be interpreted as the position (four) vector of the centre of force and the dots denote differentiations with respect to proper time. The presence of the term $\omega^2(x \, . \, \dot{x} - y \, . \, \dot{x})\dot{x}_\mu$ in the equations of motion ensures that the constraint $\dot{x}_\mu\dot{x}_\mu = -1$ (which implies $\dot{x}_\mu\ddot{x}_\mu = 0$) is consistent with the equations.

Suppose, now, that $x_\mu = (0, 0, q, t)$, $y_\mu = (0, 0, 0, t)$, then the two non-trivial equations which follow from (4.1) are identical and the dynamical system is described by the single equation

$$\frac{d^2q}{dt^2} + \omega^2 \left\{1 - \left(\frac{dq}{dt}\right)^2\right\} q = 0 \tag{4.2}$$

[Notice that we have taken the velocity of light = 1.]

Equation (4.2) is our starting point. It can be shown that equation (4.2) is the Euler–Lagrange equation following from the variation of the action $\int_{t_1}^{t_2} L \, dt$, where

$$L = m \exp(-\omega^2 q^2/2) \left\{\frac{dq}{dt} \sin^{-1}\left(\frac{dq}{dt}\right) + \left(1 - \left(\frac{dq}{dt}\right)^2\right)^{1/2}\right\} - m \tag{4.3}$$

Thus

$$\frac{\partial L}{\partial q} = -m\omega^2 q \exp(-\omega^2 q^2/2) \left\{\frac{dq}{dt} \sin^{-1}\left(\frac{dq}{dt}\right) + \left(1 - \left(\frac{dq}{dt}\right)^2\right)^{1/2}\right\}$$

$$p = \frac{\partial L}{\partial \left(\frac{dq}{dt}\right)} = m \exp\left(-\frac{\omega^2}{2} q^2\right) \sin^{-1}\left(\frac{dq}{dt}\right)$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \left(\frac{\partial q}{\partial t}\right)}\right) = m \exp(-\omega^2 q^2/2)$$

$$\times \left\{-\omega^2 q \frac{dq}{dt} \sin^{-1}\left(\frac{dq}{dt}\right) + \left(1 - \left(\frac{dq}{dt}\right)^2\right)^{-1/2} \frac{d^2q}{dt^2}\right\} \tag{4.4}$$

so that

$$\frac{d}{dt}\left(\frac{\partial L}{\partial\left(\dfrac{dq}{dt}\right)}\right)=\frac{\partial L}{\partial q}$$

coincides with equation (4.2). In order that p, L may be one-valued functions of q, dq/dt, we interpret $\sin^{-1} x$ as that value which lies in the closed interval $[-\pi/2, \pi/2]$. With this restriction $(d/dx)(\sin^{-1} x) = +\,1/\sqrt{(1-x^2)}$.

The Hamiltonian H is given by

$$\begin{aligned} H = p\frac{dq}{dt} - L &= -m \exp(-\omega^2 q^2/2)\cos\left(\frac{p}{m}\exp(\omega^2 q^2/2)\right) + m \\ &= \frac{p^2}{2m} + \tfrac{1}{2}m\omega^2 q^2 - \tfrac{1}{4}\left(\tfrac{1}{2}m\omega^4 q^4 - \omega^2 q^2\frac{p^2}{m} + \frac{1}{6}\frac{p^4}{m^3}\right) + \ldots \end{aligned} \tag{4.5}$$

Notice the interesting feature $0 \leqslant H \leqslant m$. When $dq/dt = 0, p = 0$ and $H = 0$. As $dq/dt \to \pm 1, p \to \pm m\pi/2 \exp(-\omega^2 q^2/2)$ and $H \to m$.

To apply the method, we write

$$\begin{aligned} \{\phi(H), f(p,q)\}_{\text{P.B.}} = \phi'(H)\Bigg[\sin\left(\frac{p\exp(\omega^2 q^2/2)}{m}\right)\frac{\partial f}{\partial q} \\ - \omega^2 q\left\{m\exp(-\omega^2 q^2/2)\cos\left(\frac{p\exp(\omega^2q^2/2)}{m}\right)\right. \\ \left. + p\sin\left(\frac{p\exp(\omega^2q^2/2)}{m}\right)\right\}\frac{\partial f}{\partial p}\Bigg] = if \end{aligned} \tag{4.6}$$

We must determine ϕ so that f is one-valued on the real phase space.

Let us introduce the variables ξ and η,

$$\begin{aligned} \xi &= \frac{1}{\omega^2}\log\cos\left(\frac{p\exp(\omega^2q^2/2)}{m}\right) + \tfrac{1}{2}q^2 \\ \eta &= \frac{1}{\omega^2}\log\cos\left(\frac{p\exp(\omega^2q^2/2)}{m}\right) - \tfrac{1}{2}q^2 \end{aligned} \tag{4.7}$$

Then

$$H = m(1 - \exp(\omega^2\eta)) \tag{4.8}$$

so that $\phi(H)$ may be regarded as a function of $\eta(\phi_1(\eta))$

$$\phi(H(\eta)) = \phi_1(\eta) \tag{4.9}$$

Equation (4.6) can now be written as

$$H'(\eta)\phi_1'(\eta)\frac{\partial f}{\partial \xi} = \tfrac{1}{2}f(\xi-\eta)^{-1/2}(\exp\,[\omega^2(\xi+\eta)]-1)^{-1/2} \tag{4.10}$$

i.e.

$$-\frac{1}{m\omega}\exp(-\omega^2\eta)\phi_1'(\eta)\frac{1}{f}\frac{\partial f}{\partial \xi} = \frac{1}{2}\frac{1}{\sqrt{(\xi^2-\eta^2)}}\psi[\omega^2(\xi+\eta)] \tag{4.11}$$

where

$$\begin{aligned}\psi(x) &= \sqrt{x}\,.\,(e^x-1)^{-1/2}\\ &= 1-\tfrac{1}{4}x+\tfrac{1}{96}x^2+\ldots\end{aligned}$$

Using the induction formulae (3.11) and collecting the terms with the multiplicative factor

$$\log\left(\frac{\xi+\sqrt{(\xi^2-\eta^2)}}{\eta}\right)$$

separately from the rest (as in Section 3) we have

$$\begin{aligned}\int \frac{1}{\sqrt{(\xi^2-\eta^2)}}\psi[\omega^2(\xi+\eta)]\,d\xi = &\left\{\psi(\omega^2\eta)+\frac{1}{2}\frac{(\omega^2\eta)^2}{2!}\psi''(\omega^2\eta)\right.\\ &\left.+\frac{3}{4}\frac{1}{2}\frac{(\omega^2\eta)^4}{4!}\psi^{(\mathrm{IV})}(\omega^2\eta)+\ldots\right\}\\ &.\log\left(\frac{\xi+\sqrt{(\xi^2-\eta^2)}}{\eta}\right)+R\end{aligned} \tag{4.12}$$

$$\begin{aligned}\frac{\xi+\sqrt{(\xi^2-\eta^2)}}{\eta} &= \frac{\dfrac{1}{\omega}\left(\log\cos\dfrac{p\exp(\omega^2q^2/2)}{m}\right)^{1/2}-\dfrac{1}{\sqrt{2}}q}{\dfrac{1}{\omega}\left(\log\cos\dfrac{p\exp(\omega^2q^2/2)}{m}\right)^{1/2}+\dfrac{1}{\sqrt{2}}q}\\ &= \frac{\omega q+i\dfrac{p}{m}+\text{higher powers}}{\omega q-i\dfrac{p}{m}+\text{higher powers}}\end{aligned} \tag{4.13}$$

The expression in { } on the right-hand side of equation (4.12) can be written as the closed form

$$\frac{1}{\pi}\int_0^{\pi}\psi[\omega^2\eta(1+\cos\theta)]\,d\theta = \frac{\omega}{\pi}\sqrt{\eta}\int_0^{\pi}(\exp[\omega^2\eta(1+\cos\theta)]-1)\,.(1+\cos\theta)^{1/2}\,d\theta. \tag{4.14}$$

Integrating (3.11) we get

$$-\frac{1}{m\omega}\exp(-\omega^2\eta)\phi_1'(\eta)\log f = \frac{1}{2}\frac{\omega}{\pi}\sqrt{\eta}\int_0^{\pi}(\exp[\omega^2\eta(1+\cos\theta)]-1)^{-1/2}\,.(1+\cos\theta)^{1/2}\,d\theta\,.\log\left(\frac{\xi+\sqrt{(\xi^2-\eta^2)}}{\eta}\,.\exp[S(\xi,\eta)]\right) \tag{4.15}$$

Bearing in mind the 'rational expansion' (4.13), we see from equation (4.15) that f is one-valued over the real phase space provided the coefficient of the logarithm on the right-hand side is equal to an integral multiple (taken as unity in the following) of that on the left-hand side, i.e.

$$\phi_1'(\eta) = -\frac{m\omega^2}{2\pi}\sqrt{\eta}\exp(\omega^2\eta)\int_0^{\pi}(\exp[\omega^2\eta(1+\cos\theta)]-1)^{-1/2}\,.(1+\cos\theta)^{1/2}\,d\theta \tag{4.16}$$

Now,

$$\phi(E) = \phi_1\left(\frac{1}{\omega^2}\log\left(1-\frac{E}{m}\right)\right)$$

so that

$$\phi'(E) = \phi_1'\left(\frac{1}{\omega^2}\log\left(1-\frac{E}{m}\right)\right).\frac{1}{\omega^2}\frac{1}{E-m}$$
$$= \frac{1}{2\pi\omega}\left\{\log\left(\frac{m}{m-E}\right)\right\}^{1/2}\,.\int_0^{\pi}\left\{1-\left(\frac{m-E}{m}\right)^{1+\cos\theta}\right\}^{-1/2}(1+\cos\theta)^{1/2}\,d\theta \tag{4.17}$$

Changing the integration variable occurring in the integral on the right-hand side of equation (4.17) by means of the transformation

$$\cos\theta = 1 - \frac{\omega^2 q^2}{\log\left(\frac{m}{m-E}\right)}$$

so that

$$\frac{1}{\omega}\left\{\log\left(\frac{m}{m-E}\right)\right\}^{1/2}(1+\cos\theta)^{1/2}\,d\theta = 4dq$$

we get

$$\phi'(E) = \frac{1}{2\pi}\,.\,4\int_0^{q_{\max}}\left(1 - \frac{(E-m)^2}{m^2}\exp(\omega^2 q^2)\right)^{-1/2} dq$$

Hence

$$\begin{aligned}\phi(E) &= \frac{1}{2\pi}\oint m\exp(-\omega^2 q^2/2)\cos^{-1}\left\{\left(\frac{m-E}{m}\right)\exp(\omega^2 q^2/2)\right\} dq\\ &= \frac{1}{2\pi}\oint p(E,q)\,dq \qquad (4.18)\end{aligned}$$

5. *The Hydrogen Atom*

The Hamiltonian is

$$H = \frac{1}{2m}\left(P_r^2 + \frac{P_\theta^2}{r^2} + \frac{P_\varphi^2}{r^2\sin^2\theta}\right) - \frac{e^2}{r} \qquad (5.1)$$

corresponding to the Hamilton–Jacobi equation for the system

$$E = \frac{1}{2m}\left[\left(\frac{\partial W}{\partial r}\right)^2 + \frac{1}{r^2}\left(\frac{\partial W}{\partial\theta}\right)^2 + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial W}{\partial\varphi}\right)^2\right] - \frac{e^2}{r} \qquad (5.2)$$

As is well known, the characteristic function W is separable and the two non-trivial constants of integration arising in the solution of W can be eliminated in favour of the action 'variables'

$$\begin{aligned}J_\varphi &= \oint\frac{\partial W(\phi)}{\partial\varphi}\,d\varphi = 2\pi P_\varphi\\ J_\theta &= \oint\frac{\partial W(\theta)}{\partial\theta}\,d\theta = 2\pi\left\{\left(P_\theta^2 + \frac{P_\varphi^2}{\sin^2\theta}\right)^{1/2} - P_\varphi\right\} \qquad (5.3)\end{aligned}$$

where $W(r,\theta,\varphi) = W(r) + W(\theta) + W(\varphi)$.

Finally, introducing the action variable J_r

$$J_r = \oint \frac{\partial W(r)}{\partial r}\, dr \tag{5.4}$$

and using the equation for $W(r)$

$$\left(\frac{\partial W(r)}{\partial r}\right)^2 + \frac{(J_\theta + J_\varphi)^2}{4\pi^2 r^2} - 2m\left(E + \frac{e^2}{r}\right) = 0 \tag{5.5}$$

one may express the energy as a function of J_r, J_θ, J_φ through the equation

$$J_r = \oint \left\{2m\left(E + \frac{e^2}{r}\right) - \frac{(J_\theta + J_\varphi)^2}{4\pi^2 r^2}\right\}^{1/2} dr \tag{5.6}$$

Explicitly,

$$E = -\frac{2\pi^2 me^4}{(J_r + J_\theta + J_\varphi)^2} \tag{5.7}$$

The system is two-fold degenerate. The frequencies ν_r, ν_θ, ν_φ are equal to

$$\nu = \frac{\partial E}{\partial J_r} = \frac{\partial E}{\partial J_\theta} = \frac{\partial E}{\partial J_\varphi} = \left(\frac{2}{\pi^2 me^4}\right)^{1/2} (-E)^{3/2} \tag{5.8}$$

(i) Let

$$\{\phi_r(H(p, q)), f\}_{\text{P.B.}(r)} = if \tag{5.9}$$

Now the modified Poisson bracket may be written as an ordinary Poisson bracket

$$\{\phi_r(H), f\}_{\text{P.B.}(r)} = \{\phi_r(H_r), f\}_{\text{P.B.}} \tag{5.10a}$$

where

$$H_r = \frac{1}{2m}\left(P_r^2 + \frac{(J_\theta + J_\varphi)^2}{4\pi^2 r^2}\right) - \frac{e^2}{r} \tag{5.10b}$$

J_θ, J_φ are to be regarded as ordinary numbers (rather than dynamical variables) when calculating the Poisson bracket on the right-hand side of equation (5.10a). Define

$$\xi = \frac{1}{2m}\left(P_r^2 + \frac{C}{r^2}\right), \qquad \text{where } C = \frac{(J_\theta + J_\varphi)^2}{4\pi^2}$$

$$\eta = H_r \tag{5.11}$$

Then equation (5.10a) may be written as

$$\phi_r'(\eta)\frac{1}{f}\frac{\partial f}{\partial \xi} = \frac{me^4}{(\xi-\eta)^2}[C(\xi-\eta)^2 - 2me^4(\xi-\eta) - 2me^4\eta]^{-1/2}$$

$$= (-2m\eta)^{-1/2}me^2\frac{1}{(\xi-\eta)^2}\left\{1 - \frac{1}{2\eta}(\xi-\eta)\right.$$

$$\left. + \left(\frac{C}{4m\eta e^4} + \frac{3}{8\eta^2}\right)(\xi-\eta)^2 + \ldots\right\} \tag{5.12}$$

On integration of (5.12) one can see that we are assured of f being one-valued over the (real) phase space provided the coefficient of the logarithmic singularity on the right-hand side is an integral multiple of that on the right-hand side, i.e.

$$n\phi_r'(\eta) = (-2m\eta)^{-3/2}m^2e^2 \tag{5.13}$$

Thus it is readily observed on comparison with equation (5.8) that

$$\phi_r'(E) = \frac{1}{n\,.\,2\pi\nu_r} \tag{5.14}$$

(ii) Now, suppose

$$\{\phi_\theta(H(p,q)), f\}_{\text{P.B.}(\theta)} = if \tag{5.15}$$

As explained above, we write

$$\{\phi_\theta(H), f\}_{\text{P.B.}(\theta)} = \{\phi_\theta(H_\theta), f\}_{\text{P.B.}}$$

where

$$H_\theta = -2\pi^2me^4\left[J_r + 2\pi\left(P_\theta{}^2 + \frac{J_\varphi{}^2}{4\pi^2\sin^2\theta}\right)^{1/2}\right]^{-2} \tag{5.16}$$

Define

$$\eta = \tfrac{1}{2}\left(P_\theta{}^2 + \frac{C_1}{\sin^2\theta}\right), \qquad \text{where } C_1 = \frac{J_\varphi{}^2}{4\pi^2}$$

$$\xi = \cot\theta, \tag{5.17}$$

so that

$$H = -\tfrac{1}{2}me^4[C_2 + \sqrt{(2\eta)}]^{-2}, \qquad C_2 = \frac{J_r}{2\pi} \tag{5.18}$$

Then equation (5.15) may be written as

$$\phi_\theta'(H)H'(\eta)\frac{1}{f}\frac{\partial f}{\partial \xi} = (C_2)^{-1/2}\frac{1}{(\xi^2+1)\left(\xi^2+1-\dfrac{2\eta}{C_2}\right)} \tag{5.19}$$

Integration of equation (5.19) then gives

$$\phi_\theta'(H)H'(\eta)\log f = \frac{1}{\sqrt{(2\eta)}}\log\left\{\frac{\left(\xi^2+1-\dfrac{2\eta}{C_2}\right)^{1/2}+\xi\left(\dfrac{2\eta}{C_2}\right)^{1/2}}{\left(\xi^2+1-\dfrac{2\eta}{C_2}\right)^{1/2}-\xi\left(\dfrac{2\eta}{C_2}\right)}\right\}$$

$$+ \text{arbitrary function of } \eta. \tag{5.20}$$

Thus the requirement of one-valuedness of f over the real phase space gives the condition

$$n\phi_\theta'(H)H'(\eta) = \frac{1}{\sqrt{(2\eta)}} \tag{5.21}$$

Now, from equation (5.18)

$$H'(\eta) = (-2mH)^{3/2}\frac{1}{m^2e^2\sqrt{(2\eta)}} \tag{5.22}$$

so that from equations (5.21), (5.22) and (5.8)

$$\phi_\theta'(H) = \frac{1}{n}m^2e^2(-2mH)^{-3/2} = \frac{1}{n\,.\,2\pi\nu_\theta} \tag{5.23}$$

(iii) Finally, suppose

$$\{\phi_\varphi(H(p,q)), f\}_{\text{P.B.}(\varphi)} = if \tag{5.24}$$

where

$$\{\phi_\varphi(H), f\}_{\text{P.B.}(\varphi)} = \{\phi_\varphi(H_\varphi), f\}_{\text{P.B.}} \tag{5.25}$$

$$H_\varphi = -2\pi^2me^4\,[J_r + J_\theta + 2\pi P_\varphi]^{-2} \tag{5.26}$$

Thus

$$\frac{\partial H_\varphi}{\partial P_\varphi} = (-2mH_\varphi)^{3/2}\cdot\frac{1}{m^2e^2} \tag{5.27}$$

and equation (5.24) may be written as

$$\phi_\varphi'(H_\varphi)\,.\,(-2mH_\varphi)^{3/2}\frac{1}{m^2e^2}\frac{\partial f}{\partial\varphi} = if \tag{5.28}$$

The one-valuedness condition is, therefore,

$$\phi_\varphi'(H_\varphi) = (-2mH)^{-3/2}m^2e^2\frac{1}{n} = \frac{1}{n\,.\,2\pi\nu_\varphi} \tag{5.29}$$

6. *Concluding Remarks*

The original motivation for this investigation arose from a study of the logical gaps in the transition from classical to quantum mechanics. Historically, the Bohr–Sommerfeld quantisation rules of the old quantum theory have played a very crucial role in the development of quantum mechanics. Through the application of the Bohr correspondence principle at the level of canonical coordinates and momenta, Born & Jordan (1925) derived the well-known commutation relations from these rules. It is, however, well known that the Bohr–Sommerfeld quantisation rules are unambiguous only when formulated in terms of dynamical variables which make the Hamilton–Jacobi equation separable (if such variables exist). Thus the 'derivation' of the commutation relations is incomplete. In the subsequent development of the subject this circumstance tended to be ignored. Rather, the emphasis was shifted to the treatment of non-periodic motions and the consequent development in the interpretation of dynamical variables as operators on a Hilbert space, originated by Born & Wiener (1925–26). Thus the straightforward generalisation of these commutation relations to the usual equal-time commutation relations for an interacting field involves a big logical gap. An interacting field cannot in general be regarded as the limiting case of a (Hamilton–Jacobi) separable system. In view of these considerations a revival of interest in the Bohr–Sommerfeld quantisation rules is worthwhile. Also, one must bear in mind that the derivation of the commutation relations for p's and q's is one special instance of the application of Bohr's general philosophy embodied in the correspondence principle. If one would introduce the correspondence principle at a level more directly accessible to experiment (e.g. for currents) one may thereby introduce a lot of formal simplicity into the theory.

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