The Quantum Poisson Bracket and Transformation Theory in Quantum Mechanics: Dirac's Early Work in Quantum Theory

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1. Introduction

P A M Dirac's discovery of the fundamental equations of quantum theory has been seen as one of the deepest insights of the human mind into the ways in which nature works. It has allowed the formulation of the fundamental laws of nature in a manner which is as clear and compact as it is beautiful. An examination of his earliest published work on the subject which appeared in the *Proceedings of the Royal Society of London* in the years 1925 and 1926 leaves the reader, even today, more than seventy-five years after their publication, captivated by the force of argument and the clarity of presentation.

Dirac's formulation of the fundamental equations of quantum mechanics may, arguably, be seen as independent of the earlier work of Heisenberg, Born and Jordan and of the subsequent work of Schrödinger. It is more abstract than either of the other two, although we now know of the equivalence of all three versions of quantum theory. While Heisenberg was certainly the first to observe the lack of commutativity in the rule for multiplication of dynamical variables in his new quantum mechanics – a rule intuited by Heisenberg from the combination rule for spectral frequencies and the Bohr correspondence principle – he did not delve deeply into the meaning and consequences of this lack of commutativity. Indeed, he went on to study the anharmonic oscillator which required $(x^2)_{mn}$ and $(x^3)_{mn}$, etc. in terms of $(x)_{mn}$, a study in which the lack of commutativity does not play a crucial role. Dirac, unlike the new quantum physicists on the Continent, was much less enamoured of the

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correspondence principle, which he felt was vague and did not lead to precise equations. Instead, he found the lack of commutativity of products of dynamical variables much more intriguing. Having relished the beauty of the Hamiltonian formulation and the power of Hamiltonian methods in classical mechanics and observed its use by Sommerfeld in atomic systems, he was expecting some kind of connection between the new dynamics and the older Hamiltonian dynamics, at least one which would show up in the limit of large quantum numbers. In the event, the connection he discovered is of universal validity, and showed a connection between classical and quantum theory based on an equation devoid of the 'imprecision' in the Bohr version of the correspondence principle.

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2.The Heisenberg Product: Quantum Differentiation

Dirac starts his considerations with a multiply periodic system with u degrees of freedom which, for the coordinate x at time t has the multiple Fourier expansion

$$\begin{aligned} x &= \sum_{\alpha_1\alpha_2\ldots\alpha_u} x(\alpha_1 \; ..\alpha_u) \; \exp i(\alpha_1\omega_1 + \quad + \alpha_u\omega_u)t \\ &= \sum_\alpha x_\alpha \; \exp i(\alpha\,\omega)t. \end{aligned} \quad (1)$$

The x_α and the coefficients $(\alpha\,\omega)$ are to be obtained classically by substitution in the equations of motion. There exist a u fold ∞ of solutions, each for a set of constants $\kappa_1 \quad . \kappa_u$: x_α and $(\alpha\omega)$ are now functions of $\kappa_1 \quad . \kappa_u$ and may be written as $x_{\alpha(\kappa)}$ and $(\alpha\,\omega)_\kappa$. In the classical theory, the rule of composition of two harmonic components relates to the same set of κs and is simple:

$$\begin{aligned} (\alpha\,\omega)_\kappa + (\beta\,\omega)_\kappa &= (\alpha+\beta,\omega)_\kappa & (2) \\ (xy)_{\alpha(\kappa)} &= \sum_r x_{r(\kappa)} y_{\alpha(\kappa)-r(\kappa)} = (y\,x)_{\alpha(\kappa)}. & (3) \end{aligned}$$

In presenting the quantum situation, Dirac begins with the prescription of Heisenberg. With no equation of motion to fall back on, one assumes the xs and ωs in quantum theory to depend on integer pairs $x(n\,m), \omega(n\,m), n = n_1 \quad . n_u$, and similarly for m. The differences $n_r - m_r, r = 1 \; .. \quad . u$ correspond to the preceding αs, but Dirac asserted that neither the ns nor any function of the ns and ms play the role of the classical κs, pointing out to which particular component a specific harmonic belongs. The quantum solutions are, Dirac asserted, all interlocked and must be considered as a whole. The rule of composition Dirac took from Heisenberg:

$$\begin{aligned} \omega(n, n-\alpha) + \omega(n-\alpha, n-\alpha-\beta) &= \omega(n, n-\alpha-\beta) \\ \text{i.e.,} \quad \omega(n,m) + \omega(m,k) &= \omega(n,k) \qquad (4) \end{aligned}$$

and for the position amplitudes:

$$\begin{aligned} (x+y)(n,m) &= x(n,m) + y(n,m) \qquad (5) \\ xy(n,m) &= \sum_k x(n,k)y(k,m) \neq yx(n,m). \qquad (6) \end{aligned}$$

Taking over such a non-commutative product rule ('the Heisenberg product') Dirac addressed the problem of the quantum equations of motion. Here, he was willing to take over the classical equations, provided the order of products could be correctly decided and provided the quantum equations could be obtained by algebraic processes not involving the interchange of factors in a product and by differentiation or integration with respect to a parameter (say t): in particular, the expression for the energy or the Hamiltonian could be taken over.

However, this did not solve the quantum problem. What of the quantum conditions? This he likened to the equations of the form:

$$\frac{\partial E}{\partial \kappa_r} = \frac{\omega_r}{2\pi}$$

allowing the identification of the κ_r with the action variables, J_r. In identifying the quantum equations it became necessary to consider quantum differentiation in general. Given that the most general quantum operation $\frac{d}{dv}$ (i.e., the differentiation being performed with respect to a possible quantum variable) satisfy the requirements of linearity and the Liebnitz law:

$$\frac{d}{dv}(x+y) = \frac{dx}{dv} + \frac{dy}{dv} \tag{7}$$

$$\frac{d}{dv}(xy) = \frac{dx}{dv}y + x\frac{dy}{dv} \tag{8}$$

he proposed the most general relation linearity demands, preserving the order of factors in a product

$$\frac{dx}{dv}(n,m) = \sum_{n'm'} a(nm;n'm')\,x\,(n'm') \tag{9}$$

with the coefficient $a(nm;n'm')$ carrying a set of four integer arguments. Eq(8) for the derivative of the product is used to put a series of constraints on the as when the arguments satisfy various equalities or inequalities leading to the following results:

$$\begin{aligned} a(nm;n'm) &= a(nk;n'k) \\ a(nk';nk) \equiv a(kk') &= -a(km;k'm) \\ a(nm;nm) &= a(mm) - a(nn) \end{aligned}$$

leading finally to the result

$$\frac{dx}{dv}(nm) = \sum_k \{x(nk)a(km) - a(nk)x(km)\} \tag{10}$$

$$\frac{dx}{dv} = xa - ax. \tag{11}$$

This is an important result for it is from this that Dirac obtains the quantum Poisson Bracket and its relation with the classical one.

3. Dirac's Version of the Correspondence Principle: the Quantum Poisson Bracket

To what, in classical theory, does the expression $(xy - yx)$, where x and y are dynamical variables or functions of dynamical variables, correspond? Suppose $x(n, n-\alpha)$ varies slowly with n, the ns being large numbers while the αs are small. Put

$$x(n, n-\alpha) \equiv x_{\alpha\kappa}, \tag{12}$$

where $n_r = \kappa_r h$ or $(\kappa_r + \alpha_r)h$, these being approximately equal. Dirac considers a typical term in the expression $xy - yx$ viz. $x(n, n-\alpha)\, y\,(n-\alpha-\beta) - y(n, n-\beta)\, x\,(n-\beta, n-\beta-\alpha)$ and after simple algebraic manipulations shows the quantity to equal

$$(\Delta x_{\alpha\kappa} y_{\beta\kappa})_{\Delta n=\beta} - (\Delta y_{\beta\kappa} x_{\alpha\kappa})_{\Delta n=\alpha} =$$

$$\sum_r \left\{ \Delta n_r \left(\frac{\Delta x_{\alpha\kappa}}{\Delta n_r}\right)_{\Delta n_r=\beta_r} y_{\beta\kappa} - \Delta n_r \left(\frac{\Delta y_{\beta\kappa}}{\Delta n_r}\right)_{\Delta n_r=\alpha_r} x_{\alpha\kappa} \right\}$$

and since $\Delta\kappa_r = h\Delta n_r$

$$= \sum_r h \left\{ \beta_r \left(\frac{\partial x_{\alpha\kappa}}{\partial \kappa_r}\right) y_{\beta\kappa} - \alpha_r \left(\frac{\partial y_{\beta\kappa}}{\partial \kappa_r}\right) x_{\alpha\kappa} \right\} \tag{13}$$

In classical theory, for a multiply periodic system, if W_r are the angle variables $= \omega_r \frac{t}{2\pi}$ we have $\frac{\partial}{\partial W_r}\{y_\beta \exp(i\,\beta_r\,\omega_r\,t)\} = 2\pi\, i\,\beta_r\, y_\beta \exp(i\,\beta\,\omega\,t)$.

The (n, m) component of $(xy - yx)$ then corresponds, in the classical theory, to

$$- \frac{ih}{2\pi} \sum_{\alpha+\beta=n-m} \sum_r$$

$$\left[\frac{\partial}{\partial \kappa_r}\{x_\alpha \exp(i\,\alpha\,\omega\,)t\}\frac{\partial}{\partial W_r}\{y_\beta \exp(i\,\beta\,\omega\,)t\}\right.$$

$$\left. - \frac{\partial}{\partial \kappa_r}\{y_\beta \exp(i\,\beta\,\omega\,)t\}\frac{\partial}{\partial W_r}\{x_\alpha \exp(i\,\alpha\,\omega\,)t\}\right]$$

Dirac is thus led to the conclusion that the difference between the Heisenberg products of two quantum dynamical variables equals $ih/2\pi$ times their classical Poisson Bracket expression.

i.e., $(xy - yx)$ corresponds to

$$-\frac{ih}{2\pi}\sum_r\left\{\left(\frac{\partial x}{\partial \kappa_r}\right)\left(\frac{\partial y}{\partial W_r}\right)-\left(\frac{\partial y}{\partial \kappa_r}\right)\left(\frac{\partial x}{\partial W_r}\right)\right\} \quad (14)$$

If we set $\kappa_R = J_r$ the action variables conjugate to W_r the classical expression for $(xy - yx)$ becomes $\frac{ih}{2\pi}$ times the classical Poisson Bracket

$$[x,y]_{cl.PB} = \sum_r\left\{\left(\frac{\partial x}{\partial W_r}\right)\left(\frac{\partial y}{\partial J_r}\right)-\left(\frac{\partial y}{\partial W_r}\right)\left(\frac{\partial x}{\partial J_r}\right)\right\}$$

$$= \sum_r\left\{\left(\frac{\partial x}{\partial p_r}\right)\left(\frac{\partial y}{\partial q_r}\right)-\left(\frac{\partial y}{\partial p_r}\right)\left(\frac{\partial x}{\partial q_r}\right)\right\} \quad (15)$$

where p_r,q_r are any set of conjugate canonical variables. Dirac is thus led to the conclusion that the difference between the Heisenberg products of two quantum dynamical variables equals $\frac{ih}{2\pi}$ times their classical Poisson Bracket expression:

$$xy - yx = \frac{ih}{2\pi}[x,y]_{cl.PB}.$$

It is then easily checked that the expression on the left satisfies the algebraic properties of the classical Poisson Bracket, in particular the Jacobi identity

$$[x,[y,z]\,]_{qu} + [z,[x,y]\,]_{qu} + [y,[z,x]\,]_{qu} = 0, \text{ where}$$

$$[x,y]_{qu} = (xy - yx)\frac{1}{i\hbar}, \quad (16)$$

which is well known to be obeyed by the classical Poisson Bracket (15).

This result obtained by Dirac for the 'Heisenberg product' from the Heisenberg–Born–Jordan combination rule and a careful analysis of the relationship with the Hamiltonian dynamics of multiply periodic systems is the first of Dirac's major contributions to the fundamentals of quantum mechanics. It provides the most elegant formulation of the correspondence principle meant to signify the transition from classical to quantum theory and can scarcely be bettered in brevity and clarity. The fundamental quantum commutation relations follow:

$$[q_r, p_s] = i\hbar\, \delta_{rs}, \; [q_r, q_s] = [p_r, p_s] = 0. \qquad (17)$$

While identical commutation relations are to be found in the Born and Jordan paper (*Z. f. Phys*, 34 (1925)) received on Sept 27, 1925 whereas Dirac's paper was received for publication in the *Proceedings of the Royal Society of London* on Nov 7, 1925 Dirac's development of the general quantum-classical dynamical connection has proved to be one of the deepest insights into the differences between the classical and quantum descriptions of nature and has proved to be of the greatest utility in subsequent theoretical developments. In particular, the time development of dynamical variables expressed in classical and quantum theories as

$$\frac{dx}{dt} = [x, H]_{cl} \; ; \; \frac{dx}{dt} = [x, H]_{qu},$$

where H is the Hamiltonian function retain the same forms in Dirac's version of the theory.

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4. Developments in Notation: the Transformation Theory

The next major contribution of Dirac, which included an important contribution to notation, was a paper entitled 'The Physical Interpretation of Quantum Dynamics' received for publication in the *Proceedings of the Royal Society*, London on Dec 2, 1926. In this paper, Dirac laid out the general principles of the new theory in a form which has survived. While his ingenious and elegant notation of bras and kets for states, dynamical variables, matrix elements, etc. does not appear in this paper in the version currently in use, the precursor to it can be seen in a form described "as an attempt to simplify the notation a little" This is also the paper in which Dirac introduces and uses the δ function extensively. He rediscovers the Schrödinger equation as a differential equation which is satisfied by the particular transformation function which carries one from the description in which the coordinate variables are diagonal to one in which such is the case with the Hamiltonian function. The range of ideas is wide and covers the physical interpretation of the theory in terms of probabilities and probability densities related to experiments. The results presented in this paper are deep and far reaching.

The paper begins with matters of notation. The matrix representing a dynamical variable g may be labeled by any set of constants of the motion, e.g. the value of a time varying coordinate at a particular instant of time. These are ordinary numbers (c-numbers). If these are $\alpha, \alpha', \alpha''$ (α stands collectively for the set $\alpha_1, \quad , \alpha_u$ for a system with u degrees of freedom) then $g \equiv g(\alpha', \alpha'')$. α', α'', etc. may take on values in a discrete set or in the continuum or in both: Dirac considers the case of the continuum as being the more general. Matrix multiplication then is written

$$ab(\alpha', \alpha'') = \int a(\alpha', \alpha''')\, d\alpha''' b\,(\alpha''', \alpha'') \qquad (18)$$

$d\alpha''' \equiv d\alpha_1''' \quad . d\alpha_u'''$ necessarily runs over the entire range of the parameters. Introducing the δ function the unit matrix is written as

$$1(\alpha', \alpha''') = \delta(\alpha_1' - \alpha_1''') \qquad . \delta(\alpha_u' - \alpha_u''') . \qquad (19)$$

Examining the fundamental problem of Heisenberg's matrix mechanics viz. finding a diagonal Hamiltonian such that the equation of motion

$$gH - Hg + i\hbar \frac{\partial g}{\partial t} = i\hbar\, \dot{g} \qquad (20)$$

subject to the quantum conditions

$$q_r p_s - p_s q_r = i\hbar \delta_{rs} \qquad (21)$$

are satisfied, Dirac noted (as had Born, Heisenberg and Jordan) the invariance of the theory under canonical transformations of the form

$$G = b\,g\,b^{-1}, \text{where } b \text{ is any matrix} \qquad (22)$$

G satisfies the same algebraic relations as g; if g is hermitian, so is G if b and b^{-1} are conjugate imaginaries. In the notation of matrix products, (20), we have

$$G(\alpha', \alpha'') = \int\int b(\alpha', \alpha''')\, d\alpha'''\, g(\alpha''', \alpha'''')\, d\alpha'''' \; b^{-1}(\alpha'''', \alpha''). \qquad (23)$$

Since permutations of the rows of G accompanied by identical permutations of the columns may be made without altering the matrix in any way, there is no 1-1 correspondence between the rows and columns of the original and transformed matrices. Thus a better notation is

$$G(\xi', \xi'') = \int\int b(\xi', \alpha')\, d\alpha'\, g(\alpha', \alpha'')\, d\alpha''\, b^{-1}(\alpha'', \xi'') \qquad (24)$$

with the ξs having no connection with the αs except that they run over the same ranges. This labelling of the matrices ensures that

$$\begin{aligned} \xi_r\,(\xi', \xi'') &= \xi'_r\, \delta(\xi'_1 - \xi''_1) \qquad \cdot\, \delta(\xi'_u - \xi''_u) \\ &= \xi'_r\, \delta(\xi' - \xi''). \end{aligned} \qquad (25)$$

Simplifying the notation further, Dirac notes that since g and G represent the same dynamical variable in different schemes the same letter may be used for them; the change of schemes may be made explicit only in their arguments. The letters b and b^{-1} connecting the two schemes are also unnecessary:

$$g\,(\xi', \xi'') = \int (\xi' \,|\, \alpha')\, d\alpha'\, g(\alpha', \alpha'')\, d\alpha''\, (\alpha'' \,|\, \xi''). \qquad (26)$$

We see in this equation the appearance of the bra-ket notation which Dirac later developed in his treatise 'The

Principles of Quantum Mechanics'. In this notation we would write (26) as

$$\langle \xi' \mid g \mid \xi'' \rangle = \int \int d\alpha' \, d\alpha'' \; \langle \xi' \mid \alpha' \rangle \, \langle \alpha' \mid g \mid \alpha'' \rangle \, \langle \alpha'' \mid \xi'' \rangle . \tag{27}$$

Where for conjugate variables Dirac writes

$$\begin{aligned} \xi \, (\xi', \xi'') &= \xi' \, \delta(\xi' - \xi'') \\ \eta \, (\xi', \xi'') &= -i \, \hbar \, \delta'(\xi' - \xi'') \end{aligned}$$

we would write, in his later notation,

$$\begin{aligned} \langle \xi' \mid \xi \mid \xi'' \rangle &= \xi' \, \delta(\xi' - \xi'') \\ \langle \xi' \mid \eta \mid \xi'' \rangle &= -i \, \hbar \, \delta'(\xi' - \xi'') \end{aligned} \tag{28}$$

and, more generally,

$$\langle \xi' \mid \eta^n \mid \xi'' \rangle = (-i \, \hbar)^n \, \delta^{(n)}(\xi' - \xi''). \tag{29}$$

Having devised a notation which satisfied his general requirements, Dirac considers the properties of the transformation functions. From the equation

$$\begin{aligned} \eta(\xi', \alpha') &= \int \eta \, (\xi', \xi'') \, d\xi'' \, (\xi'' \mid \alpha') \\ &= -i \, \hbar \int \delta'(\xi' - \xi'') \, d\xi'' \, (\xi'' | \alpha') \\ \text{one has } \eta(\xi', \alpha') &= -i \, \hbar \, \frac{\partial}{\partial \xi'} (\xi' \mid \alpha'). \end{aligned} \tag{30}$$

If one has an arbitrary function of ξ

$$f(\xi) \, (\xi', \alpha') \equiv \langle \xi' \mid f(\xi) \mid \alpha' \rangle = f(\xi') \, (\xi' \mid \alpha'). \tag{31}$$

Similarly, one has

$$f(\xi, \eta) \, (\xi', \alpha') = f\left(\xi', -i \, \hbar \frac{\partial}{\partial \xi'}\right) \, (\xi' \mid \alpha'). \tag{32}$$

This formula is now used to obtain a matrix representation that makes any specified function of the dynamical variables diagonal. Suppose one has a function $F(\xi, \eta)$ which we want to diagonalize in a matrix scheme,i.e.,

$$\langle \alpha' \mid F \mid \alpha'' \rangle = F(\alpha', \alpha'') = F(\alpha')\, \delta(\alpha' - \alpha'')$$

then for the appropriate transformation function we have the differential equation

$$F\left(\xi', -i\hbar \frac{\partial}{\partial \xi'}\right) (\xi' \mid \alpha') = F(\alpha')\, (\xi' \mid \alpha'), \qquad (33)$$

which is an ordinary differential equation for $(\xi' \mid \alpha')$ considered as a function of the ξ's: its solutions are to be specified for different values of the parameters αs. The eigenvalues of the differential equation, denoted by $F(\alpha')$ are the elements of the diagonal matrix for F If the ξ and η are the ordinary q and p and F is the ordinary Hamiltonian function, then this equation is just the ordinary Schrödinger wave equation and $F(\alpha')$ are the energy eigenvalues. In this way Dirac shows that the eigenfunctions of the Schrödinger equation may be viewed as the transformation functions i.e. the elements of the transformation matrix that enable the transformation from the scheme in which the qs are diagonal to one in which the Hamiltonian is diagonal.

5. Conclusion

In the preceding an attempt has been made to give in outline the genesis and development of ideas relating to two of Dirac's most important contributions to the foundations of quantum theory. These are amongst his earliest contributions but they already exemplify the directness and simplicity of his thought, combined with a search for beauty and elegance in the associated mathematical formalism. His success in this search for the foundations of physical theory expressed in equations which are, at once, simple and beautiful may be measured by the seminal influence exercised over generations of physicists by his description of the new mechanics in 'The Principles of Quantum Mechanics'

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