NATIONAL BUREAU OF STANDARDS REPORT

2188

QUANTUM DYNAMICS

Part I

by

Julian Schwinger

U. S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

U. S. DEPARTMENT OF COMMERCE
Charles Sawyer, *Secretary*

NATIONAL BUREAU OF STANDARDS
A. V. Astin, *Director*

THE NATIONAL BUREAU OF STANDARDS

The scope of activities of the National Bureau of Standards is suggested in the following listing of the divisions and sections engaged in technical work. In general, each section is engaged in specialized research, development, and engineering in the field indicated by its title. A brief description of the activities, and of the resultant reports and publications, appears on the inside of the back cover of this report.

Electricity. Resistance Measurements. Inductance and Capacitance. Electrical Instruments. Magnetic Measurements. Applied Electricity. Electrochemistry.

Optics and Metrology. Photometry and Colorimetry. Optical Instruments. Photographic Technology. Length. Gage.

Heat and Power. Temperature Measurements. Thermodynamics. Cryogenics. Engines and Lubrication. Engine Fuels. Cryogenic Engineering.

Atomic and Radiation Physics. Spectroscopy. Radiometry. Mass Spectrometry. Solid State Physics. Electron Physics. Atomic Physics. Neutron Measurements. Infrared Spectroscopy. Nuclear Physics. Radioactivity. X-Rays. Betatron. Nucleonic Instrumentation. Radiological Equipment. Atomic Energy Commission Instruments Branch.

Chemistry. Organic Coatings. Surface Chemistry. Organic Chemistry. Analytical Chemistry. Inorganic Chemistry. Electrodeposition. Gas Chemistry. Physical Chemistry. Thermochemistry. Spectrochemistry. Pure Substances.

Mechanics. Sound. Mechanical Instruments. Aerodynamics. Engineering Mechanics. Hydraulics. Mass. Capacity, Density, and Fluid Meters.

Organic and Fibrous Materials. Rubber. Textiles. Paper. Leather. Testing and Specifications. Polymer Structure. Organic Plastics. Dental Research.

Metallurgy. Thermal Metallurgy. Chemical Metallurgy. Mechanical Metallurgy. Corrosion.

Mineral Products. Porcelain and Pottery. Glass. Refractories. Enameled Metals. Concreting Materials. Constitution and Microstructure. Chemistry of Mineral Products.

Building Technology. Structural Engineering. Fire Protection. Heating and Air Conditioning. Floor, Roof, and Wall Coverings. Codes and Specifications.

Applied Mathematics. Numerical Analysis. Computation. Statistical Engineering. Machine Development.

Electronics. Engineering Electronics. Electron Tubes. Electronic Computers. Electronic Instrumentation.

Radio Propagation. Upper Atmosphere Research. Ionospheric Research. Regular Propagation Services. Frequency Utilization Research. Tropospheric Propagation Research. High Frequency Standards. Microwave Standards.

Ordnance Development.
Electromechanical Ordnance.
Electronic Ordnance.
These three divisions are engaged in a broad program of research and development in advanced ordnance. Activities include basic and applied research, engineering, pilot production, field testing, and evaluation of a wide variety of ordnance matériel. Special skills and facilities of other NBS divisions also contribute to this program. The activity is sponsored by the Department of Defense.

Missile Development. Missile research and development: engineering, dynamics, intelligence, instrumentation, evaluation. Combustion in jet engines. These activities are sponsored by the Department of Defense.

● Office of Basic Instrumentation ● Office of Weights and Measures.

NATIONAL BUREAU OF STANDARDS REPORT

NBS PROJECT		NBS REPORT
1101-10-5100	December 19, 1952	2188

QUANTUM DYNAMICS

Part I

by

Julian Schwinger

University of California, Los Angeles

and

Harvard University

PREPRINT

*This work was performed on a National Bureau of Standards contract with the University of California, Los Angeles, and was sponsored (in part) by the Office of Naval Research, USN.

NBS

ACKNOWLEDGMENT

This material was presented in a series of lectures during my visit to the National Bureau of Standards in the summer of 1952. I should like to thank Stephen Gasiorowicz and Walter Futterman, whose careful lecture notes served as a basis for this paper. Part II, which deals with perturbation theory, will be ready in the near future.

Julian Schwinger

Quantum Dynamics*
Part I

by Julian Schwinger**

Quantum Mechanics developed historically as a set of "quantization rules" superimposed upon the structure of Classical Mechanics. In view of the fact that the laws of classical physics are only limiting laws, it seems advisable to construct a self-contained quantum theory. The development of quantum dynamics to be outlined in the following lectures will parallel the development of classical mechanics from the action principle of Hamilton but will not be built upon it. In addition to improving the logical basis of quantum mechanics, the theory provides powerful general methods for the solution of problems. The discussion will be confined to systems of particles, the extension to fields (i.e., systems with an infinite number of degrees of freedom) following analogously.

We shall start with the mathematical foundation which will not be the usual geometrical basis involving vectors in Hilbert spaces, etc. We shall develop instead an algebraic basis which is in somewhat closer correspondence with the physical phenomena to be described, and is constructed as a symbolic representation of the measuring process in the atomic domain with its characteristic statistical features.

---

*This work was performed on a National Bureau of Standards contract with the University of California, Los Angeles, and was sponsored (in part) by the Office of Naval Research, USN.

**University of California, Los Angeles, and Harvard University.

I. The Algebra of Measurement

A measurement may be considered as a process by which an assembly of systems is "sorted" into sub-assemblages characterized by the same set of numbers representing the property being measured (e.g., the Stern-Gerlach experiment). Thus if we intend to "measure" the property A whose possible values are a', a'', ... (denoted generally by a') then we symbolically represent by $M(a')$ the measuring process which out of an assembly of systems selects those, for which the property A has the values a'. The measuring process $M(a')$ has the following properties:

(i) Reproducibility: If a certain measurement is followed by a second measurement of the same property then the results of the previous measurement are repeated. This is symbolically represented by

$$M(a')M(a') = M(a') \tag{1.1}$$

(ii) Exclusiveness: If we make a measurement of the property A and look for the sub-assemblage having the numbers a', and then make a measurement upon this sub-assemblage and look for systems having the values $a''(a'' \neq a')$ for A then we will expect to find no such systems and this is symbolically represented by

$$M(a')M(a'') = 0 \tag{1.2}$$

where 0 stands for the measurement process that selects no system. The properties (i) and (ii) may be combined to give

$$M(a')M(a'') = \delta(a', a'')M(a') \tag{1.3}$$

in which the numbers 1 and 0 represent certainty and impossibility of agreement respectively, for the results of the two measurements.

(iii) Completeness: If we look for all possible values of A, every system in the assembly will fall somewhere in that classification, and we then can write symbolically

$$\sum_{a'} M(a') = 1 \tag{1.4}$$

where 1 stands for the measurement process that selects all systems. It follows from (1.3) that

$$\sum_{a''} M(a')M(a'') = \sum_{a''} M(a'')M(a') = M(a')$$

so that one can consistently ascribe to 1 the algebraic property of the unit element.

More precisely, we mean by measurement the determination of the values of the maximum number of simultaneously determinable quantities, and we take a' to represent the set of numbers corresponding to such a complete measurement. We speak of a system so selected as being in the state characterized by a'. This measurement process is one that selects systems in a particular state and leaves them in that state. A more general measuring process is one which selects systems in the state a', say, and leaves them in the different state a'' associated with the same set of properties A. Such a process is symbolically denoted by $M(a', a'')$. In this notation, the previous simple measurement corresponds to $M(a'a')$. Clearly

$$M(a'a'')M(a'''a'''') = \delta(a'', a''')M(a'a'''') \quad . \tag{1.5}$$

An even more general measuring process is one in which systems with properties A characterized by the set of numbers a' are selected, and are then left in the state characterized by the numbers b' for the property B, where B and A are not simultaneously determinable. Such a measuring process is symbolized by $M(a'b')$. Clearly we have

$$M(a'b')M(b''c') = \delta(b', b'')M(a'c') \quad . \tag{1.6}$$

The question now is: What can we say about

$$M(a'b')M(c'd')$$

This must be proportional to $M(a'd')$, since the sequence of measurements takes us from a' to d'. The constant of proportionality is 1 when $c' = b'$, and 0 when $c' = b'' \neq b'$. In general we know that the state c' cannot be predicted if the system is known to be in the state b'. In fact we get the whole spectrum of values of c', each value having a certain probability. Pending a more quantitative probability interpretation we denote the numerical constant of proportionality in the above relation by $(b'|c')$, and so write

$$M(a'b')M(c'd') = (b'|c')M(a'd') \quad . \tag{1.7}$$

In particular

$$(b'|b'') = \delta(b', b'') \quad . \tag{1.8}$$

We see that the algebra defined by the measuring process and the associated numbers is linear, associative and non-commutative. The last two properties can easily be shown to be true since

$$M(a'b')[M(c'd')M(e'f')] = M(a'b')(d'|e')M(c'f')$$

$$= (d'|e')(b'|c')M(a'f')$$

while

$$[M(a'b')M(c'd')]M(e'f') = (b'|c')M(a'd')M(e'f')$$

$$= (b'|c')(d'|e')M(a'f')$$

also

$$M(a'b')M(c'd') = (b'|c')M(a'd')$$

$$M(c'd')M(a'b') = (d'|a')M(c'b') \neq (b'|c')M(a'd') \quad .$$

We shall now obtain some consequences of this algebra. Thus when

$$M(a')M(b'c')M(d') = (a'|b')(c'|d')M(a'd')$$

is summed over a' and d', then by virtue of (1.4) we get

$$M(b'c') = \sum_{a'd'}(a'|b')(c'|d')M(a'd') \tag{1.9}$$

which is a linear relation giving the connection between two sets of measurement symbols. In particular if B and C are the same physical quantities, and $b' = c'$, then

$$M(b') = \sum_{a'd'}(a'|b')(b'|d')M(a'd')$$

If we now also take A and D to represent the same set of physical quantities, we then get

$$M(b') = \sum_{a'a''} (a'|b')(b'|a'')M(a'a'') \quad .$$

Now taking

$$M(a')M(b')M(c') = (a'|b')(b'|c')M(a'c')$$

summing over b' and using (1.4) we get

$$M(a')M(c') = \left(\sum_{b'} (a'|b')(b'|c')\right) M(a'c')$$

or $$(a'|c')M(a'c') = \left(\sum_{b'} (a'|b')(b'|c')\right) M(a'c')$$

so that we infer the numerical relation

$$(a'|c') = \sum_{b'} (a'|b')(b'|c') \quad . \tag{1.10}$$

If we specialize this to the case where A = C we then get

$$\sum_{b'} (a'|b')(b'|a'') = \delta(a', a'') \tag{1.11}$$

<u>The Trace</u>

It follows from (1.10) that

$$(c'|b') = \sum_{d'a'} (c'|d')(d'|a')(a'|b') \quad . \tag{1.12}$$

This, together with (1.9) leads to the result that

$$M(b'c') - (c'|b') = \sum_{a'd'} (a'|b')(c'|d') \left(M(a'd') - (d'|a')\right) \quad . \tag{1.13}$$

This indicates that if we associate some number with $M(b'c')$ in a linear manner, the choice $M(b'c') \longrightarrow (c'|b')$ will be invariant under the transformation (1.9)

We call the associated number the <u>trace</u> of $M(b'c')$, so that

$$\mathrm{Tr.}\, M(b'c') = (c'|b') \quad . \tag{1.14}$$

We now deduce some properties of the trace:

We find that

$$\begin{aligned} \mathrm{Tr.}\, M(c'd')M(a'b') &= \mathrm{Tr.}\, (d'|a')M(c'b') \\ &= (d'|a')\, \mathrm{Tr.}\, M(c'b') \\ &= (d'|a')(b'|c') \quad . \end{aligned}$$

Similarly we have

$$\mathrm{Tr.}\, M(a'b')M(c'd') = (b'|c')(d'|a')$$

so that the trace of a product of two measuring symbols is independent of the order of the multiplicants.

As a consequence of (1.8) we have

$$\mathrm{Tr.}\, M(a'a'') = \delta(a', a'') \tag{1.15}$$

and

$$\mathrm{Tr.}\, M(a') = 1 \quad .$$

In addition we have the relation that

$$\mathrm{Tr.}\, M(a')M(b') = (a'|b')(b'|a') \quad . \tag{1.16}$$

The Adjoint

The measurement symbol $M(a'b')$ as written implies a certain sense, namely the succession of events happens as read from left to right. The measurement symbol in which the convention is opposite to the above one is called the adjoint symbol, and is denoted by $M(a'b')^{+}$, where

$$M(a'b')^{+} \equiv M(b'a') \quad . \tag{1.17}$$

As a result of this definition

$$\begin{aligned}(M(a'b')M(c'd'))^{+} &= M(d'c')M(b'a') \\ &= M(c'd')^{+}M(a'b')^{+} \quad .\end{aligned} \tag{1.18}$$

This can also be written as

$$[(b'|c')M(a'd')]^{+} = (c'|b')M(a'd')^{+} \tag{1.19}$$

so that with a reversal in sense $(b'|c')$ is replaced by $(c'|b')$. If we insist that no physical result depend upon this convention, the probability of transition between states a' and b' must involve $(a'|b')$ and $(b'|a')$ symmetrically. A quantity possessing the correct properties is

$$p(a', b') = p(b', a') = (a'|b')(b'|a') \tag{1.20}$$

$$\sum_{b'} p(a', b') = 1$$

where the latter statement, which follows from (1.11), is of course

necessary for any probability interpretation. However, a probability must also be a real non-negative number. If $(a'|b')$ is considered to be defined in the field of complex numbers, this will be satisfied by the following restriction on the measuring algebra,

$$(b'|a') = (a'|b')^* \tag{1.21}$$

i.e.,

$$p(a', b') = |(a'|b')|^2 \geq 0 \quad .$$

Note the general algebraic property of the adjoint operation deduced from (1.19) and (1.21)

$$[(b'|c')M(a'd')]^+ = (b'|c')^* M(a'd')^+ \quad .$$

Operators and Matrices

A symbol can be associated with a physical quantity in the following way. We have from (1.16) and (1.20) that

$$\mathrm{Tr.}\ M(a')M(b') = p(a', b') \tag{1.22}$$

hence we obtain for the expectation value of the physical quantity B in the state a'

$$\langle B \rangle_{a'} = \sum_{b'} b' p(a', b') = \mathrm{Tr.}\ BM(a') \tag{1.23}$$

where

$$B = \sum_{b'} b' M(b') \quad . \tag{1.24}$$

Other forms follow from

$$M(b') = \sum_{a'a''} (a'|b')(b'|a'')M(a'a'') = \sum_{a'c'} (a'|b')(b'|c')M(a'c')$$

i.e.,

$$B = \sum (a'|B|a'')M(a'a'') = \sum (a'|B|c')M(a'c') \tag{1.25}$$

where

$$(a'|B|a'') = \sum_{b'} (a'|b')b'(b'|a'') = \text{Tr. } BM(a''a') \tag{1.26}$$

$$(a'|B|c') = \sum_{b'} (a'|b')b'(b'|c') = \text{Tr. } BM(c'a') \quad .$$

Thus a physical quantity is characterized in relation to an arbitrary measuring process by an array of numbers — a matrix. From the general relation between measurement symbols

$$M(d'a') = \sum_{b'c'} (a'|b')M(c'b')(c'|d') \tag{1.27}$$

we deduce the matrix transformation law,

$$(a'|X|d') = \sum_{b'c'} (a'|b')(b'|X|c')(c'|d') \tag{1.28}$$

with the aid of the trace formula (1.26).

For the product of two quantities we have, say

$$XY = \sum (a'|X|b')M(a'b') \sum (b''|Y|c')M(b''c')$$

$$= \sum (a'|X|b')(b'|Y|c')M(a'c')$$

or

$$(a'|XY|c') = \sum_{b'} (a'|X|b')(b'|Y|c'), \tag{1.29}$$

the matrix multiplication law. In view of the complete correspondence between the measurement algebra and the conventional mathematical formulation, we shall borrow the usual terminology. Thus we call the elements of the algebra operators, etc. We have anticipated this connection in speaking of the trace. Thus according to our definition

$$\text{Tr. } B = \sum_{b'} b' = \sum_{a'} (a'|B|a') \quad . \tag{1.30}$$

Note also our definition of the adjoint of an operator

$$X = \sum (a'|X|b')M(a'b')$$

namely

$$X^{+} = \sum (a'|X|b')^{*}M(b'a') \tag{1.31}$$

shows that

$$(b'|X^{+}|a') = (a'|X|b')^{*} \quad . \tag{1.32}$$

Since the symbols of elementary measurements, $M(a')$ are self-adjoint (Hermitian)

$$M(a')^{+} = M(a') \tag{1.33}$$

this property extends to the operator representing any physical quantity, i.e., one with real eigenvalues.

Eigenvectors

The measurement symbol $M(a'b')$, describing the transition of a system from the state a' to the state b', can be analyzed further by introducing a hypothetical state of non-existence, 0. Thus we may think of a two-step process equivalent to $M(a'b')$,

$$M(a'b') = M(a'0)M(0b')$$

where $M(a'0)$ symbolizes a measurement which selects systems in the state a' and annihilates them, while $M(0b')$ describes the creation of a system in the state b'. We shall use the notation

$$M(a'0) = \Psi(a') \tag{1.34}$$

$$M(0a') = \Psi(a')^{+}$$

so that

$$M(a'b') = \Psi(a')\Psi(b')^{+} \quad . \tag{1.35}$$

The algebraic properties of the adjoint operator then correctly yield

$$M(a'b')^{+} = \Psi(b')\Psi(a')^{+} = M(b'a') \quad .$$

According to the multiplication law

$$M(0a')M(b'0) = (a'|b')M(0)$$

or

$$\Psi(a')^{+}\Psi(b') = (a'|b')M(0) \quad . \tag{1.36}$$

Thus,

$$(a'|b') = (0|\Psi(a')^{+}\Psi(b')|0) \tag{1.37}$$

or with a simplified notation, in which the null state is understood,

$$(a'|b') = (\Psi(a')^{+}\Psi(b')) \quad . \tag{1.38}$$

In particular

$$(\Psi(a')^{+}\Psi(a'')) = \delta(a', a'') \quad . \tag{1.39}$$

We infer from (1.38) that

$$(a'|b')^{*} = (\Psi(b')^{+}\Psi(a')) = (b'|a')$$

and from (1.37) that

$$(a'|b') = \mathrm{Tr.}\,\Psi(a')^{+}\Psi(b') = \mathrm{Tr.}\,\Psi(b')\Psi(a')^{+}$$

$$= \mathrm{Tr.}\, M(b'a') \quad .$$

For a general operator represented by

$$X = \sum (a'|X|b')\Psi(a')\Psi(b')^{+}$$

we deduce that

$$X\Psi(b') = \sum_{a'} \Psi(a')(a'|X|b') \tag{1.40}$$

and

$$\Psi(a')^{+} X = \sum_{b'} (a'|X|b')\Psi(b')^{+}$$

since

$$\Psi(a')M(0) = \Psi(a'), \; M(0)\Psi(b')^{+} = \Psi(b')^{+} \quad . \tag{1.41}$$

In particular, justifying the eigenvector designation,

$$A\Psi(a') = a'\Psi(a')\Psi(a')^{+}A = \Psi(a')^{+}a' \quad .$$

We can also conclude from (1.40) that

$$\Psi(a')^{+}X\Psi(b') = (a'|X|b')M(0) \tag{1.42}$$

whence

$$(a'|X|b') = (\Psi(a')^{+}X\Psi(b')) \tag{1.43}$$

and

$$(a'|X|b') = \mathrm{Tr.}\,\Psi(a')^{+}X\Psi(b')$$

$$\mathrm{Tr.}\; XM(b'a') \quad .$$

As a special case of the measurement symbol transformation equation (1.9) we have

$$M(b'0) = \sum_{a'}(a'|b')M(a'0); \; M(0a') = \sum_{b'}(a'|b')M(0b')$$

or

$$\Psi(b') = \sum_{a'}\Psi(a')(a'|b'); \; \Psi(a')^{+} = \sum_{b'}(a'|b')\Psi(b')^{+} \tag{1.44}$$

in which the transition amplitudes $(a'|b')$ appear most directly as

transformation functions. Conversely the transformation equation (1.9) follows from (1.44). Note also the converse derivation of the multiplication law,

$$M(a'b')M(c'd') = \Psi(a')\Psi(b')^{+}\Psi(c')\Psi(d')^{+}$$

$$\Psi(a')(\Psi(b')^{+}\Psi(c'))\Psi(d')^{+}$$

$$(b'|c')M(a'd')$$

which involves (1.41).

Unitary Transformations

We now look more precisely at the changes in the manner of description of our system. Consider two descriptions of the system, one in terms of the properties A, with eigenvalues a', the other in terms of the properties B with eigenvalues b'. Since the number of independent states of the system is the same in A as in B, we can establish a one-to-one correspondence between the states a' and b'. After making the association $a' \longleftrightarrow b'$ we take M(a'b') to refer to pairs of states put in such a one-to-one correspondence. We now define the quantity

$$U_{ab} \equiv \sum_{\substack{\text{all pairs} \\ (a'b')}} M(a'b') \quad . \tag{1.45}$$

Evidently

$$U_{aa} = \sum_{a'} M(a') = 1 \tag{1.46}$$

and

$$U_{ba} = \sum_{(a'b')} M(b'a') = U^{+}_{ab} \quad . \tag{1.47}$$

For sequence transformations $a \longrightarrow b \longrightarrow c$, we have

$$U_{ab}\, U_{bc} = \sum_{(a'b')} M(a'b') \sum_{(b'c')} M(b'c') \tag{1.48}$$

$$= \sum_{a'c'} M(a'c') = U_{ac}$$

where the c' written down is the one corresponding to the a' through the intermediary of b'.

In particular with $c = a$, we have

$$U_{ab}\, U_{ba} = 1 \tag{1.49}$$

and similarly,

$$U_{ba}\, U_{ab} = 1 \tag{1.50}$$

so that

$$U_{ab}\, U^{+}_{ab} = U^{+}_{ab}\, U_{ab} = 1 \tag{1.51}$$

which characterizes U_{ab} as a unitary operator.

It follows from the definition of U_{ab} that

$$U_{ab}\Psi(b') = \Psi(a') \quad , \quad \Psi(a')^{+}U_{ab} = \Psi(b')^{+} \tag{1.52}$$

where a' and b' are corresponding states.

The inverse relations are

$$U_{ba}\Psi(a') = \Psi(b') \quad , \quad \Psi(b')^{+}U_{ba} = \Psi(a')^{+} \qquad (1.53)$$

One can construct the transformation function $(a'|b'')$ as a matrix element of the operator U_{ba} in the 'a' description

$$\begin{aligned}(a'|b'') &= (\Psi(a')^{+}\Psi(b'')) = (\Psi(a')^{+}U_{ba}\Psi(a'')) \\ &= (a'|U_{ba}|a'')\end{aligned} \qquad (1.54)$$

or the 'b' description,

$$\begin{aligned}(a'|b'') &= (\Psi(a')^{+}\Psi(b'')) = (\Psi(b')^{+}U_{ba}\Psi(b'')) \\ &= (b'|U_{ba}|b'') \ .\end{aligned} \qquad (1.55)$$

We now remark that

$$M(b') = U_{ba}M(a')U_{ab} \qquad (1.56)$$

which follows directly from the multiplication law of the measurement symbols, or from the eigenvector construction

$$M(b') = \Psi(b')\Psi(b)^{+} = U_{ba}\Psi(a')\Psi(a')^{+}U_{ab} \ . \qquad (1.57)$$

Accordingly,

$$\begin{aligned}B &= \Sigma\, b'M(b') = U_{ba}\,\Sigma\, b(a')\,M(a')\,U_{ab} \\ &= U_{ba}\,b(A)\,U_{ab}\end{aligned} \qquad (1.58)$$

where the correspondence between eigenvalues enters in writing b' as a function of the corresponding eigenvalue a'. We have also used the general definition of a function of an operator,

$$b(A) = \sum_{a'} b(a')\, M(a') \quad . \tag{1.59}$$

In the important situation where A and B have the same spectrum, we can establish the correspondence so that

$$a' = b' \tag{1.60}$$

and therefore

$$B = U_{ba}\, A\, U_{ab} \ , \qquad A = U_{ab}\, B\, U_{ba} \tag{1.61}$$

Conversely, let U be an arbitrary unitary operator $U^{+} = U^{-1}$, and construct

$$\bar{A} = UAU^{-1} = \sum a'\, UM(a')U^{-1} \quad . \tag{1.62}$$

This can be written

$$\bar{A} = \sum \bar{a}'\, M(\bar{a}')$$

where

$$\bar{a}' = a'$$

and

$$\Psi(\bar{a}') = U\Psi(a') \ , \quad \Psi(\bar{a}')^{+} = \Psi(a')^{+}\, U^{-1} \ ,$$
$$(\Psi(\bar{a}')^{+}\Psi(\bar{a}'')) = \delta(\bar{a}',\bar{a}'') \tag{1.63}$$

so that $\bar{A}$ and A possess the same eigenvalue spectrum and corresponding eigenvectors are related by the operator U.

For an arbitrary operator

$$X = \Sigma\, (a' |X| a'')\, M(a'a'')$$

we have

$$\bar{X} = U X U^{-1} = \Sigma\, (a' |X| a'')\, M(\bar{a}'\bar{a}'')$$

so that

$$(\bar{a}' |\bar{X}| \bar{a}'') = (a' |X| a'') \quad . \tag{1.64}$$

Furthermore, all algebraic relations are preserved,

$$\overline{(X + Y)} = \bar{X} + \bar{Y} \quad , \quad (\bar{X}\bar{Y}) = \overline{XY}$$

and

$$(\bar{X})^{+} = \overline{(X^{+})} \quad .$$

Thus the description resulting from the unitary transformation is on precisely the same footing as the original description.

<u>Infinitesimal Unitary Transformations</u>

Consider the special situation in which $\bar{A}$ and A differ infinitesimally, as obtained from a unitary operator U which is in the infinitesimal neighborhood of the unit operator:

$$U = 1 - \frac{i}{\hbar} F \quad . \tag{1.65}$$

Here F is an infinitesimal operator and $\hbar$ is introduced as a constant with the dimensions of action in order that our physical quantities be measured in conventional units. Since U is unitary, we must have

$$U^{+} = 1 + \frac{i}{\hbar} F^{+}$$

equal to

$$U^{-1} = 1 + \frac{i}{\hbar} F \quad ,$$

that is, F must be an infinitesimal Hermitian operator. We write

$$\Psi(\bar{a}') - \Psi(a') = (U - 1)\ \Psi(a') \equiv \delta\Psi(a') \tag{1.66}$$

so that

$$\delta\Psi(a') = -\frac{i}{\hbar} F \Psi(a') \tag{1.67}$$

and

$$\delta\Psi(a')^{+} = \frac{i}{\hbar}\ \Psi(a')^{+} F \quad . \tag{1.68}$$

For an arbitrary operator X,

$$\bar{X} = U X U^{-1} = X + \frac{i}{\hbar} [X,F] \quad .$$

This we write as

$$\bar{X} = X - \delta X \tag{1.69}$$

where

$$\frac{1}{i\hbar} [X,F] = \delta X \quad . \tag{1.70}$$

Now it follows from (1.64) that

$$(\bar{a}'|X|\bar{a}'') - (a'|X|a'') = (\bar{a}'|X - \bar{X})|\bar{a}'') \quad . \tag{1.71}$$

For an infinitesimal transformation this becomes, in our notation,

$$\delta(a'|X|a'') = (a'|\delta X|a'') \tag{1.72}$$

where the operator is held fixed on the left side.

An important special case is that in which it is possible to construct δA as an arbitrary infinitesimal multiple of the unit operator,

$$\delta A = \delta a$$

which requires that

$$[A, (F/\delta a)] = i\hbar \quad . \tag{1.73}$$

Since

$$\bar{A}\Psi(\bar{a}') = (A - \delta a)\Psi(\bar{a}') = a'\Psi(\bar{a}')$$

yields

$$A\Psi(\bar{a}') = (a' + \delta a)\Psi(\bar{a}') \quad ,$$

which implies that $\Psi(\bar{a}')$ is an eigenvector of A with the eigenvalue $a' + \delta a$, our assumption can be realized only when A possesses a continuous spectrum. Notice that (1.72) reads

$$\delta(a'|A|a'') = \delta a \, \delta(a', a'')$$

in agreement with the fact that the change in the eigenvectors is equivalent to increasing the eigenvalues by δa.

We now examine the effect on a transformation function $(a'|b')$ (a' and b' again refer to arbitrarily chosen eigenvalues) of subjecting the 'a' states to an infinitesimal unitary transformation generated by F_a, and the 'b' states to an independent transformation generated by F_b. Since

$$(a'|b') = (\Psi(a')^{+} \Psi(b'))$$

we get

$$\delta(a'|b') = \frac{i}{\hbar}(\Psi(a')^{+} F_a \Psi(b')) - \frac{i}{\hbar}(\Psi(a')^{+} F_b \Psi(b'))$$

or

$$\delta(a'|b') = \frac{i}{\hbar}(a'|(F_a - F_b)|b') \quad . \tag{1.74}$$

Of course, if the same transformation is applied to both types of states ($F_a = F_b$), the transformation function is unaltered.

One may inquire, more generally, what form $\delta(a'|b')$ must have, for any conceivable alteration that is consistent with the three fundamental properties of transformation functions, namely

$$\sum_{b'}(a'|b')(b'|c') = (a'|c') \quad ,$$

$$(a'|a'') = \delta(a',a'') \quad , \tag{1.75}$$

$$(a'|b')^{*} = (b'|a') \quad .$$

We shall write

$$\delta(a'|b') = \frac{i}{\hbar}(a'|\delta W_{ab}|b') \tag{1.76}$$

which is the definition of the infinitesimal operator δW_{ab}. According to the first, composition property, changes in $(a'|b')$ and $(b'|c')$ imply a change in $(a'|c')$ given by

$$\delta(a'|c') = \Sigma\, \delta(a'|b')(b'|c') + \Sigma(a'|b')\,\delta(b'|c')$$

$$= \frac{i}{\hbar}\Sigma\, (a'|\delta W_{ab}|b')(b'|c') + \frac{i}{\hbar}\Sigma\, (a'|b')(b'|\delta W_{bc}|c')$$

$$= \frac{i}{\hbar}(c'|(\delta W_{ab} + \delta W_{bc}|c')$$

which is the additive composition property

$$\delta W_{ab} + \delta W_{bc} = \delta W_{ac} \quad . \tag{1.77}$$

In particular, if $c = a$, we have from the second fundamental property,

$$\delta W_{ab} + \delta W_{ba} = 0 \quad . \tag{1.78}$$

The third general property of transformation function implies that

$$-\frac{i}{\hbar}(a'|\delta W_{ab}|b')^* = \frac{i}{\hbar}(b'|\delta W_{ba}|a')$$

or

$$\delta W_{ab}^{\,+} = -\delta W_{ba}$$

$$= \delta W_{ab} \quad , \tag{1.79}$$

that is, δW_{ab} is an infinitesimal Hermitian operator. Of course these conditions are satisfied by the special form

$$\delta W_{ab} = F_a - F_b \quad . \tag{1.80}$$

II. The Dynamical Principle

We introduce the time t as a parameter upon which physical quantities depend, and require (principle of time homogeneity) that all values of t be equivalent, for complete physical systems. This means that the spectrum of a physical quantity is independent of t, and that a change of t corresponds to a unitary transformation. Furthermore, we assert that, in general, compatible physical quantities refer to the same time. That is, a state (of maximum information) will be specified by the values of a complete set of quantities at a given time, $\xi(t)$. We write the associated eigenvector as $\Psi(\xi' t)$. A change in description may consist of choosing a new set of commuting operators at the time t, or of changing the time for a given set of commuting operators, or of both alterations. Thus the most general transformation function is

$$(\xi_1' t_1 | \xi_2'' t_2) = (\Psi(\xi_1' t_1)^{+} \Psi(\xi_2'' t_2)) \quad . \qquad (2.1)$$

This describes the relation between states at the two times and thus contains the entire dynamical history of the system in this interval. It is the object of quantum dynamics to construct all such transformation functions, and accordingly, we may expect that the fundamental dynamical principle will be a differential characterization of this general transformation function.

According to the work of the last section, we know that for any change of the transformation function (2.1), be it of the times t_1

and t_2, of the operators ζ_1 and ζ_2, or of the physical attributes of the system in the interval from t_1 to t_2, that

$$\delta(\zeta_1' t_1 | \zeta_2'' t_2) = \frac{1}{\hbar}(\zeta_1' t_1 | \delta W_{12} | \zeta_2'' t_2) \quad , \qquad (2.2)$$

where δW_{12} is an infinitesimal Hermitian operator with the additive property

$$\delta W_{12} + \delta W_{23} = \delta W_{13} \quad .$$

Another additivity property refers to composite systems, i.e., two dynamically independent systems α and β, which are considered in conjunction. If the states of α and β are described by the eigenvectors $\Psi(\zeta^{\alpha'} t)$ and $\Psi(\zeta^{\beta'} t)$, respectively, the composite state is described by

$$\Psi(\zeta^{\alpha'} \zeta^{\beta'} t) = \Psi(\zeta^{\alpha'} t)\ \Psi(\zeta^{\beta'} t) = \Psi(\zeta^{\beta'} t)\ \Psi(\zeta^{\alpha'} t) \ .$$

Accordingly

$$(\zeta_1^{\alpha'} \zeta_1^{\beta'} t_1 | \zeta_2^{\alpha''} \zeta_2^{\beta''} t_2) = (\zeta_1^{\alpha'} t_1 | \zeta_2^{\alpha''} t_2)(\zeta_1^{\beta'} t_1 | \zeta_2^{\beta''} t_2)$$

and

$$(\zeta_1^{\alpha'} \zeta_1^{\beta'} t_1 | X^{\alpha} | \zeta_2^{\alpha''} \zeta_2^{\beta''} t_2) = (\zeta_1^{\alpha'} t_1 | X^{\alpha} | \zeta_2^{\alpha''} t_2)(\zeta_1^{\beta'} t_1 | \zeta_2^{\beta''} t_1)$$

where X^{α} is a physical quantity of the α system. There is an analogous statement for X^{β}. With the shorthand notation $(1) = (1)_{\alpha}\ (1)_{\beta}$, we find

$$\delta(1) = \delta(1)_\alpha (1)_\beta + (1)_\alpha \delta(1)_\beta$$

$$= \frac{i}{\hbar}(|(\delta W_{12}^\alpha + \delta W_{12}^\beta)|)$$

which is the additivity property for dynamically independent systems:

$$\delta W_{12}^\alpha + \delta W_{12}^\beta = \delta W_{12} \quad .$$

There are two types of infinitesimal changes in the transformation functions. In the first we adhere to a given dynamical system and introduce infinitesimal alterations of $\xi_1(t_1)$ and $\xi_2(t_2)$. This includes changes of t_1 and t_2. These transformations are generated by infinitesimal Hermitian operators, F_1 and F_2, which are functions of dynamical variables at t_1 and t_2, respectively. Hence for this type of change

$$\delta W_{12} = F_1 - F_2 \quad .$$

In the second type of change, the initial and final states are unaltered, but some physical characteristic of the system is modified in the time interval t, $t + dt$. Now

$$(\xi_1' t_1 | \xi_2'' t_2) =$$

$$\int (\xi_1' t_1 | \xi' t + dt) d\xi' (\xi' t + dt | \xi'' t) d\xi'' (\xi'' t | \xi_2'' t_2) \quad ,$$

which has been written in the form appropriate to continuous spectra. Transformation functions referring to an interval that does not include $(t, t + dt)$ will not be altered, while, as a special case of (2.2),

$$\delta(\xi' t + dt | \xi'' t) = \frac{i}{\hbar}(\xi' t + dt | \delta L(t)dt | \xi'' t)$$

where $\delta L(t)$ is an infinitesimal Hermitian function of dynamical variables at time t, and the differential dt appears to conform with the vanishing of the left side for equal times. We conclude that for this type of change,

$$\delta W_{12} = \delta L(t)dt \quad , \tag{2.3}$$

or more generally, if we consider a distribution of variations in physical attributes,

$$\delta W_{12} = \int_{t_2}^{t_1} \delta L(t)dt \quad .$$

The form of the infinitesimal operator characterizing a general change in the transformation function is then

$$\delta W_{12} = F_1 - F_2 + \int_{t_2}^{t_1} \delta L(t)dt \quad ,$$

or if we construct a function F(t) such that

$$F(t_1) = F_1 \quad , \quad F(t_2) = F_2 \quad ,$$

we may write

$$\delta W_{12} = \int_{t_2}^{t_1} \left[\frac{dF(t)}{dt} + \delta L(t) \right] dt \quad .$$

We now assume that there are classes of changes for which the generating operators δW_{12} are obtained by appropriate variation of a single operator W_{12},

$$\delta W_{12} = \delta(W_{12}) \quad ,$$

and that W_{12} has the form

$$W_{12} = \int_{t_2}^{t_1} L(t)dt$$

where $L(t)$, the Lagrangian operator, to borrow the classical terminology, is a function of certain fundamental dynamical variables x_i, in the infinitesimal neighborhood of t, i.e.,

$$L(t) = L\left(x_i(t) \quad , \quad \frac{d}{dt}\, x_i(t),\ t\right) \quad .$$

The limitation to first derivatives can always be achieved by suitable adjunctions of dynamical variables. We take L to be a Hermitian operator, thus imparting the same property to W_{12}, the action integral operator, and thereby satisfy the requirement that δW_{12} be Hermitian. As indicated by the explicit occurrence of t in the Lagrangian, our treatment will not be restricted to complete systems. One should notice, however, that for a system acted on by time dependent external forces, not every physical quantity has a time independent spectrum.

There will occur in the structure of the Lagrangian certain parameters. Any alteration of these quantities is a change in the nature of the dynamical system (the addition to a Lagrangian of a new term can be thought of in this way). The associated δW_{12},

$$\delta W_{12} = \int_{t_2}^{t_1} \delta\,(L(t))dt$$

has the form (2.3) with $\delta L = \delta(L)$. On the other hand, for a given form of the Lagrangian, we may introduce certain infinitesimal

changes of the $x_i(t)$, and of t_1 and t_2. This must correspond to the possibility of altering the nature of the states, at t_1 and t_2 for a fixed dynamical system. Hence

$$\delta W_{12} = F_1 - F_2 \quad .$$

This is the operator principle of stationary action since δW_{12} must be independent of dynamical variables in the interval between t_1 and t_2. We shall obtain therefrom equations of motion for the $x_i(t)$, and expressions for F_1 and F_2.

We may note here that if we were to replace L with

$$\bar{L} = L - \frac{d}{dt} W \quad , \qquad W = W(x(t), t)$$

or W_{12} with $\bar{W}_{12}$,

$$\bar{W}_{12} = W_{12} - (W_1 - W_2) \quad , \quad W_1 = W(t_1) \quad , \quad W_2 = W(t_2)$$

we should be adding to W_{12} operators referring to times t_1 and t_2. Hence the stationary action principle leads to the same equations of motion with $\bar{W}_{12}$ as with W_{12}, and

$$\delta \bar{W}_{12} = \bar{F}_1 - \bar{F}_2$$

where

$$\delta W_1 = F_1 - \bar{F}_1 \quad , \quad \delta W_2 = F_2 - \bar{F}_2 \quad .$$

Hence altering the Lagrangian by the addition of a time derivative does not change the dynamical system under consideration, but rather yields new generators of infinitesimal transformations at t_1 and t_2.

Concerning the structure of the Lagrangian, we require that the limitation to first derivatives be maintained under any integration by parts, i.e., the addition of a total time derivative. This implies that the Lagrangian is linear in the time derivatives. Accordingly, we write

$$L = \frac{1}{2} \Sigma\, b_{ij}\left(x_i \frac{dx_j}{dt} - \frac{dx_i}{dt} x_j\right) - H(x,t) \tag{2.4}$$

where (b_{ij}) is a numerical matrix. This structure remains unchanged if an integration by parts is performed on the time derivative terms. The operators x_i can be chosen Hermitian without loss of generality. In order that L be Hermitian, it is necessary that H, the Hamiltonian operator, be Hermitian, and that

$$\Sigma\, b_{ij}\left(x_i \frac{dx_j}{dt} - \frac{dx_i}{dt} x_j\right) = \Sigma\, b^*_{ij}\left(\frac{dx_j}{dt} x_i - x_j \frac{dx_i}{dt}\right)$$
$$= -\Sigma\, b^*_{ji}\left(x_i \frac{dx_j}{dt} - \frac{dx_j}{dt} x_i\right)$$

or

$$b_{ij} = -b^*_{ji} \quad ,$$

the b-matrix must be skew-Hermitian. We shall decompose b_{ij} into anti-symmetrical and symmetrical elements,

$$b_{ij} = a_{ij} + s_{ij} \quad ,$$

$$a_{ij} = -a_{ji} \quad , \quad s_{ij} = s_{ji}$$

which are, respectively, real and imaginary,

$$a^*_{ij} = a_{ij} \quad , \quad s^*_{ij} = -s_{ij} \quad ,$$

and assume that the dnyamical variables correspondingly decompose into two kinematically independent sets; variables of the first kind, associated with a_{ij}, and variables of the second kind, associated with $s_{\alpha\beta}$ (employing Greek indices to distinguish the second set):

$$L = \frac{1}{2} \Sigma\, a_{ij} \left(x_i \frac{dx_j}{dt} + \frac{dx_j}{dt} x_i \right) + \frac{1}{2} \Sigma\, s_{\alpha\beta} \left(x_\alpha \frac{dx_\beta}{dt} - \frac{dx_\beta}{dt} x_\alpha \right) - H(x_i, x_\alpha, t) \ .$$

We have used the phrase 'kinematically independent' to mean the decomposition of the time derivative terms, as distinguished from 'dynamically independent' which refers to an additive structure of the entire Lagrangian, i.e., of the Hamiltonian also.

The action integral associated with the Lagrangian (2.4) is

$$W_{12} = \int_{t_2}^{t_1} \left[\tfrac{1}{2} \Sigma\, b_{ij} \left(x_i dx_j - dx_i x_j \right) - H\, dt \right]$$

$$= \int_{\tau_2}^{\tau_1} \left[= \Sigma\, b_{ij} \left(x_i \frac{dx_j}{dt} - \frac{dx_i}{dt} x_j \right) - H \frac{dt}{d\tau} \right] dt \ .$$

On subjecting this to a variation we may keep the τ limits fixed, representing variations of t_1 and t_2 by an alteration of the functional relation between t and τ. Since τ is not varied we need not write it explicitly

$$\delta W_{12} = \int \left[\tfrac{1}{2} \Sigma\, b_{ij}(\delta x_i dx_j - dx_i \delta x_j + x_i d\delta x_j - d\delta x_i x_j) - \delta H\, dt - H\, d\delta t \right]$$

$$= \int d \left[\tfrac{1}{2} \Sigma\, b_{ij}(x_i \delta x_j - \delta x_i x_j) - H \delta t \right]$$

$$+ \int \left[\Sigma\, b_{ij}(\delta x_i dx_j - dx_i \delta x_j) - \delta H\, dt + dH \delta t \right] .$$

The stationary action principle requires the vanishing of the second term, which can be expressed as

$$\delta H = \frac{dH}{dt} \delta t + \Sigma\, b_{ij}(\delta x_i \frac{dx_j}{dt} - \frac{dx_i}{dt} \delta x_j)$$

$$= \frac{dH}{dt} \delta t + \Sigma\, a_{ij}(\delta x_i \frac{dx_j}{dt} + \frac{dx_j}{dt} \delta x_i) + \Sigma\, s_{\alpha\beta}(\delta x_\alpha \frac{dx_\beta}{dt} - \frac{dx_\beta}{dt} \delta x_\alpha) \quad . \tag{2.5}$$

We also obtain

$$F_1 = F(t_1) \quad , \quad F_2 = F(t_2)$$

where

$$F = \tfrac{1}{2} \Sigma\, b_{ij}(x_i \delta x_j - \delta x_i x_j) - H \delta t$$

$$= \tfrac{1}{2} \Sigma\, a_{ij}(x_i \delta x_j + \delta x_j x_i) + \tfrac{1}{2} \Sigma\, s_{\alpha\beta}(x_\alpha \delta x_\beta - \delta x_\beta x_\alpha) - H \delta t \quad . \tag{2.6}$$

The character of the variations to which the principle of stationary action refers is now made explicit by the statement that the symmetrizations and anti-symmetrizations occurring in (2.5) and (2.6) are superfluous, in virtue of the operator property of δx_i and δx_α. We infer the commutator and anti-commutator relations

$$\left[\delta x_j , x_i \right] = 0 \quad , \qquad \left\{ \delta x_\beta , x_\alpha \right\} = 0$$

$$\left[\delta x_j , \frac{dx_i}{dt} \right] = 0 \quad , \qquad \left\{ \delta x_\beta , \frac{dx_\alpha}{dt} \right\} = 0 \quad .$$

Now we shall obtain from (2.5) expressions for $\frac{dx_i}{dt}$ and $\frac{dx_\alpha}{dt}$ as functions of the dynamical variables, in terms of the structure of the Hamiltonian. The first of the latter conditions is then satisfied if

$$\left[\delta x_j , x_\alpha \right] = 0$$

which gives δx_j the character of an infinitesimal multiple of the unit operator. The second of the latter conditions is satisfied with

$$\left[\delta x_\beta , x_i \right] = 0$$

provided $\frac{dx_\alpha}{dt}$ is an odd function ot the variables of the second kind. It is thus necessary that the Hamiltonian be an even function of the variables of the second kind, but is without restriction in its dependence on the variables of the first kind.

We write

$$\delta H = \frac{\partial H}{\partial t} \quad t + \sum \delta x_i \frac{\partial H}{\partial x_i} + \sum \delta x_\alpha \frac{\partial_L H}{\partial x_\alpha} \quad ,$$

or an alternative form in which 'left derivatives' are replaced by 'right derivatives'

$$\sum \delta x_\alpha \frac{\partial_L H}{\partial x_\alpha} = \sum \frac{\partial_r H}{\partial x_\alpha} \delta x_\alpha \quad .$$

No such distinction occurs for first class variables. The equations of motion are obtained as

$$\frac{dH}{dt} = \frac{\partial H}{\delta t} ,$$

$$2 \sum_j a_{ij} \frac{dx_j}{dt} = \frac{\partial H}{\delta x_i} ,$$

$$2 \sum_\beta s_{\alpha\beta} \frac{dx_\beta}{dt} = \frac{\partial_L H}{\partial x_\alpha} = - \frac{\partial_r H}{\delta x_\alpha} ,$$

and

$$F = \sum a_{ij} x_i \delta x_j + \sum s_{\alpha\beta} x_\alpha \delta x_\beta - H \delta t .$$

We now turn our attention to variables of the first class.

The Canonical Form

In order that the equations of motion be solvable for the $\frac{dx_i}{dt}$, the anti-symmetrical matrix (a_{ij}) must be non-singular. This requires that N, the number of the x_i, be even. Indeed

$$\det a_{ij} = \det a_{ji} = (-1)^N \det a_{ij} ;$$

the determinant vanishes identically for N odd. Hence,

$$N = 2n$$

when the integer n is the number of degrees of freedom. Now a real anti-symmetrical matrix of even dimension can, by real linear transformations, be reduced to the canonical form

$$\frac{1}{2}\begin{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} & 0 & \\ 0 & \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} & \\ & & \ddots \end{pmatrix} .$$

To show this we consider the bi-linear form

$$A = \sum_{i,j=1}^{2n} a_{ij}x_i y_j = a_{12}(x_1 y_2 - x_2 y_1) + x_1 \sum_{k=3}^{2n} a_{1k} y_k + x_2 \sum_{k=3}^{2n} a_{2k} y_k$$

$$- \left\{\sum_{k=3}^{2n} a_{1k} x_k\right\} y_1 - \left(\sum_{k=3}^{2n} a_{2k} x_k\right) y_2 + \sum_{i,j=3}^{2n} a_{ij} x_i y_j \quad .$$

We assume that $a_{12} > 0$ (if it is negative, then $a_{21} > 0$ and we may satisfy our assumption by a relabeling) and define the quantities ξ_1, $\xi_{1'}$, η_1 and $\eta_{1'}$

$$(2a_{12})^{-\frac{1}{2}} \xi_1 = x_1 - \frac{1}{a_{12}} \sum_3^{2n} a_{2k} x_k$$

$$(2a_{12})^{-\frac{1}{2}} \eta_1 = y_1 - \frac{1}{a_{12}} \sum_3^{2n} a_{2k} y_k$$

$$(2a_{12})^{-\frac{1}{2}} \xi_{1'} = x_2 + \frac{1}{a_{12}} \sum_3^{2n} a_{1k} x_k$$

$$(2a_{12})^{-\frac{1}{2}} \eta_{1'} = y_2 + \frac{1}{a_{12}} \sum_3^{2n} a_{1k} y_k \quad .$$

Under this transformation A becomes

$$A = \tfrac{1}{2}(\xi_1 \eta_{1'} - \xi_{1'} \eta_1) + \sum_{i,j=3}^{2n} \left[a_{ij} - \frac{1}{a_{12}} (a_{1i}a_{2j} - a_{1j}a_{2i})\right] x_i y_j \quad .$$

Since the matrix of the 2n - 2 dimensional form is again anti-symmetrical, we can repeat this process and finally obtain

$$A = \frac{1}{2} \sum_{k=1}^{n} (\xi_k \eta_{k'} - \xi_{k'} \eta_k)$$

For the linear combinations of x_i variables associated with the canonical form we shall write

$$\xi_k = p_k \ , \quad \xi_{k'} = q_k \ , \quad k = 1, \ldots n \ .$$

Thus the Lagrangian and the infinitesimal generator F become (we are considering only the first class variables)

$$L = \frac{1}{4} \sum \left(p_k \frac{dq_k}{dt} - q_k \frac{dp_k}{dt} + \frac{dq_k}{dt} p_k - \frac{dp_k}{dt} q_k \right) - H(q, p, t) \ ,$$

$$F = \frac{1}{2} \sum (p_k \delta q_k - q_k \delta p_i) - H \delta t \ ,$$

while the equations of motion in the canonical form read

$$\frac{dq_k}{dt} = \frac{\partial H}{\partial p_k} \ , \quad \frac{dp_k}{dt} = \frac{\partial H}{\partial q_k} \ , \quad \frac{dH}{dt} = \frac{\partial H}{\partial t} \ .$$

It will be noted that the derivative terms in the Lagrangian can be given less symmetrical but simpler forms by the addition of total time derivatives. Thus

$$\frac{1}{4} \sum \left(\left\{ p_k, \frac{dq_k}{dt} \right\} - \left\{ q_k, \frac{dp_k}{dt} \right\} \right)$$
$$= \frac{1}{2} \sum \left\{ p_k, \frac{dq_k}{dt} \right\} - \frac{d}{dt} \frac{1}{4} \sum \left\{ p_k, q_k \right\}$$
$$= - \frac{1}{2} \sum \left\{ q_k, \frac{dp_k}{dt} \right\} + \frac{d}{dt} \frac{1}{4} \sum \left\{ p_k, q_k \right\}$$

and correspondingly

$$\frac{1}{2} \sum (p_k \delta q_k - q_k \delta p_k) = \sum p_k \delta q_k - \delta \left[\frac{1}{4} \sum \left\{ p_k, q_k \right\} \right]$$
$$= - \sum q_k \delta p_k + \delta \left[\frac{1}{4} \sum \left\{ p_k, q_k \right\} \right] \ .$$

Hence if we employ a form of L in which only derivatives of the q_k occur,

$$L = \frac{1}{2} \sum \left\{ p_k , \frac{dq_k}{dt} \right\} - H ,$$

that part of F referring to changes in the q_k and p_k will be

$$F_{\delta q} = \sum p_k \delta q_k ,$$

while if L contains only derivatives of the p_k,

$$L = - \frac{1}{2} \sum \left\{ q_k , \frac{dp_k}{dt} \right\} - H ,$$

the relevant part of F is

$$F_{\delta p} = - \sum q_k \delta p_k .$$

The Canonical Commutation Relations

We must evidently interpret $F_{\delta q}$ as the generator of an infinitesimal change of the q_k with no alteration of the p_k, and conversely for $F_{\delta p}$. Hence

$$\left[q_k , F_{\delta q} \right] = i \hbar \delta q_k , \quad \left[p_k , F_{\delta q} \right] = 0 ,$$

$$\left[p_k , F_{\delta p} \right] = i \hbar \delta p_k , \quad \left[q_k , F_{\delta p} \right] = 0 .$$

Since δq_k, δp_l commute with all quantities, i.e., are arbitrarily infinitesimal multiples of the unit operator, we have

$$\sum_\gamma \left[q_k, p_\gamma\right] \delta q_\gamma = i\hbar\, \delta q_k \quad , \quad \sum \left[p_k, p_\gamma\right] \delta q_\gamma = 0$$

$$-\sum_\gamma \left[p_k, q_\gamma\right] \delta p_\gamma = i\hbar\, \delta p_k \quad , \quad \sum_\gamma \left[q_k, q_\gamma\right] \delta p_\gamma = 0$$

or

$$\left[q_k, q_\gamma\right] = \left[p_k, p_\gamma\right] = 0 \quad ,$$

$$\left[q_k, p_\gamma\right] = i\hbar\, \delta_{k\gamma}$$

where the last canonical commutation relation is consistently obtained from both generators. Observe that for any change of q_k alone that is compatible with the commutation relations

$$\left[\delta q_k, q_\gamma\right] = \left[\delta q_k, p_\gamma\right] = 0 \quad ,$$

and similarly with δp_k. This is our original hypothesis concerning the δq_k are δp_k, which is thereby shown to be consistent with the commutation relations derived therefrom. It also follows from (1.72) et. seq. that the spectra of the q's and p's form a continuum.

If G(q,p) is an arbitrary function, we have

$$\left[G, F_{\delta q}\right] = i\hbar\, \delta_q G = i\hbar \sum \frac{\partial G}{\partial q_k} \delta q_k$$

or

$$\frac{\partial G}{\partial q_k} = \frac{1}{i\hbar}\left[G, p_k\right] = \frac{i}{\hbar}\left[p_k, G\right] \quad .$$

Similarly,

$$\left[G, F_{\delta p}\right] = i \hbar \, \delta_p G = i \hbar \sum \frac{\partial G}{\partial p_k} \delta p$$

yields

$$\frac{\partial G}{\partial p_k} = \frac{1}{i\hbar}\left[q_k, G\right] = \frac{i}{\hbar}\left[G, q_k\right] \quad .$$

Complete sets of compatible physical quantities (commuting operators) are provided by the totality of q's, or of p's , at the same time. Thus we have two elementary descriptions, with the associated eigenvectors $\Psi\,(q't)$ and $\Psi\,(p't)$. The transformation generated by $F_{\delta q}$ and $F_{\delta p}$ have a particularly simple aspect for these eigenvectors:

$$-\frac{i}{\hbar} F_{\delta q} \, \Psi\,(q't) = \delta_q \, \Psi\,(q't) = \sum \frac{\partial}{\partial q_k'} \Psi(q't)\, \delta q_k \quad ,$$

$$-\frac{i}{\hbar} F_{\delta p} \, \Psi\,(p't) = \delta_p \, \Psi\,(p't) = \sum \frac{\partial}{\partial p_k'} \Psi(p't)\, \delta p_k$$

whence

$$p_k \Psi(q't) = i \hbar \, \frac{\partial}{\partial q_k'} \Psi(q't)$$

$$q_k \Psi(p't) = \frac{\hbar}{i} \, \frac{\partial}{\partial p_k'} \Psi(p't) \quad .$$

The adjoint equations are

$$\Psi(\delta't)^{+} \, p_k = \frac{\hbar}{i} \, \frac{\partial}{\partial q_k'} \Psi(q't)^{+} \quad ,$$

$$\Psi\,(p't)^{+} \, q_k = i \hbar \, \frac{\partial}{\partial p_k'} \Psi(p't)^{+} \quad .$$

If $G(q,p)$ is an arbitrary function of the q's, but a polynomial in the p's, we have

$$\Psi(q't)^{+}\, G(q\, p) = G(q', \tfrac{\hbar}{i} \tfrac{\partial}{\partial q'})\ \Psi(q't)^{+} \quad .$$

This follows by induction from its assumed validity for G_1 and G_2 and its verification for $G_1 + G_2$ and for G_1G_2:

$$\Psi(q't)^{+}\, G_1(q\, p)\, G_2(q\, p) = G_1(q', \tfrac{h}{2} \tfrac{\partial}{\partial q'})\ \Psi(q't)^{+}\, G_2(q\, p)$$

$$= G_1(q', \tfrac{\hbar}{2} \tfrac{\partial}{\partial q'})\, G_2\, (q', \tfrac{\hbar}{2} \tfrac{\partial}{\partial q'})\, \Psi(q't)^{+} \quad ,$$

combined with the evident truth of the statement for $G = G(q)$, and $G = p_k$. On the other hand,

$$G(q,p)\, \Psi(q't) = \tilde{G}\, (q', i\, \hbar \tfrac{\partial}{\partial q'})\, \Psi(q't)$$

where the order of all factors is reversed in $\tilde{G}$. The significant part of the induction proof is

$$G_1(q\, p)\, G_2(q\, p)\Psi(q't) = G_1(q\, p)\, \tilde{G}_2(q', i\, \hbar \tfrac{\partial}{\partial q'})\, \Psi(q't)$$

$$= \tilde{G}_2(q', i\, \hbar \tfrac{\partial}{\partial q'})\, \tilde{G}_1(q', i\, \hbar\, \tfrac{\partial}{\partial q'})\, \Psi(q't)$$

$$= \widetilde{G_1\, G_2}\, (q', i\, \hbar \tfrac{\partial}{\partial q'})\, \Psi(q't) \quad .$$

Notice that if G is a Hermitian function of the q's and p's with real coefficients, $\tilde{G} = G$. The analogous statements for a function that is a polynomial in the q's are

$$\Psi(p't)^{+}\, G(q\, p) = G(i\hbar \frac{\partial}{\partial q'}\, ,\, p')\, \Psi(p't)^{+} \quad ,$$

$$G(q\, p)\, \Psi(p't) = \tilde{G}(\frac{\hbar}{2} \frac{\partial}{\partial p'}\, ,\, p')\, \Psi(p't) \quad .$$

Notice that the effect of $F_{\delta p}$ on $\Psi\,(q't)$, and of $F_{\delta q}$ on $\Psi\,(p't)$ is just a numerical phase change:

$$\delta_p \Psi(q't) = -\frac{i}{\hbar} F_{\delta p} \Psi(q't) = \frac{i}{\hbar}\,(\Sigma\, q_k' \delta p_k)\, \Psi(q't) \quad ,$$

$$\delta_q \Psi(p't) = -\frac{i}{\hbar} F_{\delta q} \Psi(p't) = \frac{i}{\hbar}\,(\Sigma\, p_k' \delta q_k)\, \Psi(p't) \quad .$$

This indicates that the notation $\Psi(q't)$, say, is really incomplete, since the change in phase does not alter the eigenvalue q', but does yield a different physical state.

Time Displacements

It is evident that

$$F_{\delta t} = -H\delta t$$

is the generator of the transformation which consists in replacing dynamical variables at time t by those at $t + \delta t$. Hence for the function G of $q(t)$, $p(t)$ and t, we have

$$[G,\, -H\delta t] = i\hbar\, \delta\, G$$

when δG is such that

$$\bar{G} = G - \delta G = G + \left(\frac{dG}{dt} - \frac{\partial G}{\partial t}\right) \delta t \quad ;$$

the unitary transformation has no effect upon t as it occurs explicitly in G. We infer the general equation of motion,

$$\frac{dG}{dt} = \frac{\partial G}{\partial t} + \frac{1}{i\hbar}[G, H] \quad .$$

By successively placing $G = H$, q_k, $- p_k$, we check the consistency of the theory by rederiving the equations of motion originally deduced from the action principle:

$$\frac{dH}{dt} = \frac{\partial H}{\delta t} \quad ,$$

$$\frac{dq_h}{dt} = \frac{1}{i\hbar}[q_h, H] = \frac{\partial H}{\partial p_h}$$

$$-\frac{dp_h}{dt} = \frac{1}{i\hbar}[H, p_h] = \frac{\partial H}{\partial q_h} \quad .$$

The time dependence of an eigenvector $\Psi(\zeta' t)$ is determined by

$$-\frac{i}{\hbar} F_{\delta t} \Psi(\zeta' t) = \delta_t \Psi(\zeta' t) = \frac{\partial}{\partial t} \Psi(\zeta' t)\, \delta t$$

whence

$$-i\hbar \frac{\partial}{\partial t} \Psi(\zeta' t) = H\, \Psi(\zeta' t)$$

and

$$i\hbar \frac{\partial}{\partial t} \Psi(\zeta' t)^{+} = \Psi(\zeta' t)^{+} H \quad .$$

In particular, if H is a polynomial function of the p's, we have

$$i\hbar \frac{\partial}{\partial t} \Psi(q' t)^{+} = H(q', \frac{\hbar}{i}\frac{\partial}{\partial q'}, t)\, \Psi(q' t)^{+}$$

and

$$-i\hbar \frac{\partial}{\partial t}(q' t) = \tilde{H}(q', i\hbar\frac{\partial}{\partial q'}, t)\, \Psi(q' t) \quad .$$

Accordingly if Ψ is the eigenvector of some state not involving t in its specification, the 'wave function' of that state

$$\Psi(q't) = (\Psi(q't)^{+}\Psi)$$

obeys the Schrödinger equations

$$i\hbar\frac{\partial}{\partial t}\,\psi\,(q't) = H(q', \frac{k}{2}\frac{\partial}{\partial q'}, t)\,\psi\,(q't)$$

and

$$i\hbar\frac{\partial}{\partial t}\,\psi\,(q't)^{*} = \tilde{H}(q', i\hbar\frac{\partial}{\partial q'}, t)\,\psi\,(q't)^{*}\quad .$$

When H is a real function, $\tilde{H} = H$. More generally, if Ψ is a member of a complete set of eigenvectors, $\Psi(\alpha')$, the transformation functions

$$(q't|\alpha') \equiv \psi_{\alpha'}\,(q't)\quad , \quad (\alpha'|q't) \equiv \psi_{\alpha'}\,(q't)^{*}$$

obeys the Schrödinger equations.

Canonical Transformations

We now consider in more detail the freedom of description for a given system associated with the possibility of replacing a Lagrangian L by

$$\bar{L} = L - \frac{d}{dt}W\quad ,$$

the action integral W_{12} by

$$\bar{W}_{12} = W_{12} - (W_1 - W_2)\quad ,$$

and the generating operator F by

$$\bar{F} = F - \delta W \quad .$$

We have seen that one can introduce a canonical form for F,

$$F = \Sigma\, p_k \delta q_k - H \delta t \quad ,$$

which implies the canonical commutator relations and the canonical equations of motion. We ask for the conditions under which $\bar{F}$ will preserve the canonical form, but expressed in terms of new quantities $\bar{q}_h$, $\bar{p}_h$, $\bar{H}(\bar{q}, \bar{p}, t)$, i.e.,

$$\bar{F} = \Sigma\, \bar{p}_k \delta \bar{q}_k - \bar{H} \delta t \quad .$$

This will yield the canonical form for the commutator relations and equations of motion obeyed by these new quantities.

The difference of the generating operators F and $\bar{F}$ is the variation of an operator W,

$$\delta W = \Sigma\, p_k \delta q_k - H \delta t - \Sigma\, \bar{p}_k \delta \bar{q}_k + \bar{H} \delta t \quad .$$

Thus, in terms of a function $W(q, \bar{q}, t)$, we obtain

$$p_k = \frac{\partial}{\partial q_k} W \quad , \quad -\bar{p}_k = \frac{\partial}{\partial \bar{q}_k} W$$

$$H = H + \frac{\partial}{\partial t} W \quad ,$$

as the equations defining such a canonical transformation, provided it is possible to solve without exceptions for the $\bar{q}$'s and $\bar{p}$'s.

An elementary example is provided by

$$W = \Sigma \, \frac{1}{2} \left\{ q_k, \, \bar{q}_k \right\} \quad .$$

We have

$$\delta W = \Sigma \, \bar{q}_k \, \delta \, q_k + \Sigma \, \bar{q}_k \, \delta \, q_k$$

so that

$$\bar{q}_k = p_k \quad , \quad \bar{p}_k = -q_k \quad , \quad \bar{H} = H \quad ;$$

this is the canonical transformation interchanging the q's and p's, with appropriate signs.

The general linear transformation is generated by

$$W = \frac{1}{2} \, \Sigma \left(\alpha_{ij} \, q_i \, q_j + \beta_{ij} \left\{ q_i, \, \bar{q}_j \right\} + \gamma_{ij} \, \bar{q}_i \, \bar{q}_j \right) \quad . \qquad (2.7)$$

We derive

$$p_i = \sum_j \left(\alpha_{ij} \, q_j + \beta_{ij} \, \bar{q}_j \right)$$

$$-\bar{p}_i = \sum \left(\beta_{ji} \, q_j + \gamma_{ij} \, \bar{q}_j \right)$$

or, in a matrix notation

$$p = \alpha q + \beta \bar{q} \quad , \quad -\bar{p} = \tilde{\beta} q + \gamma \bar{q} \quad .$$

The explicit equations of the transformation are then

$$\bar{q} = a \, q + b \, p$$

$$\bar{p} = c \, q + d \, p$$

where

$$a = -\beta^{-1}\alpha \quad , \qquad b = \beta^{-1}$$

$$c = -\tilde{\beta} + \gamma\beta^{-1}\alpha \quad , \quad d = -\gamma\beta^{-1} \quad .$$

The four matrices a, b, c, d satisfy the relation

$$a\,\tilde{d} - b\,\tilde{c} = 1$$

which, in fact, is just the condition that

$$[\bar{q}_k, \bar{p}_\ell] = i\,\hbar\,\delta_{k\ell} \quad .$$

The matrices appearing in W are expressed in terms of the matrices of the transformation equations by

$$\alpha = -\,b^{-1}\,a \quad , \quad \beta = b^{-1} \quad , \quad \gamma = -\,d\,b^{-1} \quad .$$

The fact that the α and γ matrices are necessarily symmetrical implies that

$$a\,\tilde{b} = b\,\tilde{\alpha} \quad , \quad \tilde{b}\,d = \tilde{d}\,b \quad , \quad c\,\tilde{d} = d\,\tilde{c} \quad ,$$

the first and third of which are the conditions on the transformation imposed by the requirements

$$[\bar{q}_k, \bar{q}_\ell] = [\bar{p}_k, \bar{p}_\ell] = 0 \quad .$$

The transformation function

$$(q't|\,\bar{q}'t) = (\Psi\,(q't)^+\;\Psi(\bar{q}'t)$$

can be constructed from the differential equation

$$\delta(q't|\bar{q}'t) = \frac{i}{\hbar}(q't|(F - \bar{F})|\bar{q}'t)$$

$$= \frac{i}{\hbar}(q't|\delta W(q,\bar{q},t)|\bar{q}'t) \quad ,$$

by performing the following process. Take the differential expression δW and, employing the commutation properties of the q's and $\bar{q}$'s, arrange the operators so that the q's everywhere stand to the left of the $\bar{q}$'s. This ordered differential expression will be denoted by $\delta\mathcal{W}(\bar{q},q,t)$. That is,

$$\delta W(q,\bar{q},t) = \delta\mathcal{W}(q,\bar{q},t) \quad ,$$

but the ordered operator $\mathcal{W}(q,\bar{q},t)$ obtained by integration is not equal to $W(q,\bar{q},t)$, and indeed is not a Hermitian operator. With this ordering, we have

$$\delta(q't|\bar{q}'t) = \frac{i}{\hbar}(q't|\delta\mathcal{W}(q,\bar{q},t)|\bar{q}'t)$$

$$= \frac{i}{\hbar}\delta\mathcal{W}(q',\bar{q}',t)(q't|\bar{q}'t)$$

since the operators now act directly on their eigenvectors. The solution of this differential equation is

$$(q't|\bar{q}'t) = e^{\frac{i}{\hbar}\mathcal{W}(q',\bar{q}',t)}$$

where the constant of integration is additively incorporated in $\mathcal{W}$. It is to be determined from normalization requirements such as

$$\int (q't|\bar{q}'t)\, d\bar{q}'(\bar{q}'t|q''t) = \delta(q' - q'') \quad . \qquad (2.8)$$

For the example of the general linear transformation we have

$$\delta W = \Sigma\ \delta q_i(\alpha_{ij}\, q_j + \beta_{ij}\, \bar{q}_j) + \Sigma\ (q_i \beta_{ij} + \bar{q}_i \gamma_{ij}) \delta \bar{q}_j = \delta \mathcal{W}\ ;$$

the ordering operation here is trivial. Hence

$$\mathcal{W} = \Sigma\ (\tfrac{1}{2}\alpha_{ij}\, q_i\, q_j + \beta_{ij}\, q_i\, \bar{q}_j + \tfrac{1}{2}\gamma_{ij}\, \bar{q}_i\, \bar{q}_j) + \text{Const.}$$

and

$$(q'|\bar{q}') = C\ (\beta)\ e^{\frac{i}{\hbar}\Sigma(\frac{1}{2}\alpha_{ij}q_i'q_j' + \beta_{ij}q_i'\bar{q}_j' + \frac{1}{2}\gamma_{ij}\bar{q}_i'\bar{q}_j')}\ ,$$

in which we have anticipated that the integration constant does not depend upon the matrices α and γ. Notice that the inverse transformation is obtained from the substitutions $q, p \leftrightarrow \bar{q}, \bar{p}$; $\alpha \leftrightarrow -\gamma$; $\beta \leftrightarrow -\tilde{\beta}$, so that

$$(\bar{q}'|q') = C(-\tilde{\beta})\ e^{-\frac{i}{\hbar}\Sigma(\frac{1}{2}\alpha_{ij}q_i'q_j' + \beta_{ij}q_i'\bar{q}_j' + \gamma_{ij}\bar{q}_i'\bar{q}_j')}\ .$$

This should also be the complex conjugate of the original transformation function, which is indeed true if

$$C(-\tilde{\beta}) = C(\beta)^*\ .$$

We now compute

$$\int (q'|\bar{q}')\ d\,\bar{q}'(\bar{q}'|q'') = |C(\beta)|^2\ e^{\frac{i}{\hbar}\,\frac{1}{2}\Sigma\alpha_{ij}(q_i'q_j' - q_i''q_j'')}\ \cdot$$

$$\cdot \int d\,\bar{q}'\ e^{\frac{i}{\hbar}\Sigma\,\beta_{ij}(q_i' - q_i'')\bar{q}_j'}$$

$$= |C(\beta)|^2\ \frac{(2\pi\hbar)^n}{|\det \beta|}\ \delta(q' - q'')$$

whence

$$|c(\beta)|^2 = \frac{|\det \beta|}{(2\pi\hbar)} \quad .$$

The condition (2.8) is now satisfied with

$$c(\beta) = \left[\left(\frac{i}{2\pi\hbar}\right)^n \det \beta \right]^{\frac{1}{2}} \quad .$$

The explicit appearance of i is demanded by the requirement that in the limit of the identity transformation, the transformation function approach $\delta(q' - \bar{q}')$. In this limit, $\alpha \to -\beta$, $\gamma \to -\beta$, $\beta^{-1} \to 0$, and

$$(q'|\bar{q}') \to \left[\left(\frac{i}{2\pi\hbar}\right)^n \det \beta \right]^{\frac{1}{2}} e^{-\frac{i}{2\hbar}\Sigma \beta_{ij}(q_i'-\bar{q}_i')(q_j'-\bar{q}_j')} \to \delta(q' - \bar{q}')$$

as it should. For the special case provided by $\bar{q}_h = p_h$, $\bar{p}_h = -q_h$, we have $\alpha = \gamma = 0$, $\beta = 1$, so that

$$(q'|p') = \left(\frac{i}{2\pi\hbar}\right)^{m/2} e^{\frac{i}{\hbar}\Sigma q_k' p_k'} \quad .$$

A simple connection between the Hermitian operator W and the non-Hermitian ordered operator $\mathcal{W}$ can be established by treating $\hbar$ as a variable parameter. We must then write the differential characterization of a transfor mation function as

$$\delta(1) = i\left(\left|\delta\left(\frac{1}{\hbar} W\right)\right|\right)$$

whence

$$(\partial/\partial \tfrac{1}{\hbar})(1) = i(|W|)$$

provided W does not involve $\hbar$ explicitly. However, the ordering process that lefines ,

$$\delta(\tfrac{1}{\hbar}\mathcal{W}) = \delta(\tfrac{1}{\hbar}W)$$

introduces $\hbar$ into the structure of $\mathcal{W}$, so that

$$W = (\partial/\partial \tfrac{1}{\hbar})(\tfrac{1}{\hbar}\mathcal{W})$$

$$= \mathcal{W} - \hbar \frac{\partial}{\partial \hbar}\mathcal{W} .$$

For the example of the general linear transformation

$$\mathcal{W} = \sum(\tfrac{1}{2}\alpha_{ij}q_i q_j + \beta_{ij}q_i\bar{q}_j + \tfrac{1}{2}\gamma_{ij}\bar{q}_i\bar{q}_j) + \frac{\hbar}{2i}\log\left[\left(\frac{i}{2\pi\hbar}\right)^n \det\beta\right] ,$$

which is non-Hermitian:

$$\mathcal{W} - \mathcal{W}^+ = -\sum\beta_{ij}\left[\bar{q}_j, \bar{q}_i\right] - i\hbar\log\frac{\det\beta}{(2\pi\hbar)^n}$$

$$= i\hbar\, n(\log 2\pi\hbar + 1) - i\hbar\log\det\beta ,$$

according to the commutation relation

$$\left[\bar{q}_k, q_l\right] = \frac{\hbar}{i}(\beta^{-1})_{kl} . \tag{2.9}$$

Now

$$\hbar\frac{\partial\mathcal{W}}{\partial\hbar} = \frac{\hbar}{2i}\log\left[\left(\frac{i}{2\pi\hbar}\right)^n \det\beta\right] + i\hbar\frac{n}{2}$$

so that

$$\mathcal{W} - \hbar \frac{\partial \mathcal{W}}{\partial \hbar} = \sum \left(\tfrac{1}{2}\alpha_{ij} q_i q_j + \beta_{ij} q_i \bar{q}_j + \tfrac{1}{2}\gamma_{ij} \bar{q}_i \bar{q}_j\right) - i\hbar \frac{n}{2}$$

which is indeed equal to W in virtue of the commutator (2.9).

<u>The Hamilton-Jacobi Transformation</u>

A canonical transformation - the Hamilton-Jacobi transformation - is generated by the action integral itself. If we put $W = W_{12}$ and write $t_1 = t$, $t_2 = t_o$, where t_o is an arbitrary <u>fixed</u> time, we have

$$\delta W = F - F_o \quad ,$$

that is,

$$\bar{F} = F_o = \sum p_k(t_o)\, \delta q_k(t_o) \quad .$$

Accordingly, the action integral induces a canonical transformation from $q_n(t)$, $p_h(t)$, $H(t)$ to $q(t_o)$, $p(t_o)$, 0. The vanishing of the new Hamiltonian is required by the fact that the new canonical variables are independent of t. Thus, the equations describing this canonical transformation are

$$p_k = \frac{\partial W}{\partial q_k} \quad , \quad -p_k(t_o) = \frac{\partial W}{\partial q_k}(t_o)$$

$$H(q, p, t) + \frac{\partial W}{\partial t} = 0 \quad ,$$

the Hamilton-Jacobi equations. Incidentally, the new Hamiltonian, $\bar{H} = 0$, should not be confused with $H(t_o)$ which determines the dependence of W on t_o,

$$\frac{\partial W}{\partial t_o} = H(q(t_o), p(t_o), t_o) \quad .$$

A simple illustration is provided by the system of one degree of freedom $H = p^2/2m$. This is a conservative system, so that W depends only on $t - t_o$, and we shall place $t_o = 0$. The equations of motion have the solution

$$q(t) = q_o + \frac{t}{m} p_o \quad , \quad p(t) = p_o$$

which is a linear transformation. Accordingly the action integral operator has the value

$$W = \frac{1}{2}\left\{q - q_o, p_o\right\} - \frac{p_o^2}{2m} t = \frac{m}{2t} (q - q_o)^2$$

which is of the general form (2.7) with

$$\alpha = \gamma = - \beta = \frac{m}{t} \quad .$$

Thus we have the commutation relation

$$[q_o, q] = i\hbar \frac{t}{m} \quad ,$$

the ordered operator

$$\mathcal{W} = \frac{m}{2t} \left(q^2 - 2q\, q_o + q_o^2\right) + \frac{i\hbar}{2} \log \left(2\pi \hbar i \frac{t}{m}\right)$$

and the transformation function

$$(q't|q''0) = e^{\frac{i}{\hbar}\mathcal{W}(q',q'',t)} = \left(\frac{m}{2\pi \hbar i t}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}\frac{m}{2t}(q'-q'')^2}$$

which satisfies the requirement

$$(q'0|q''0) = \delta(q' - q'') \quad .$$

It is often convenient to employ $p_k(t_o)$ rather than $q_k(t_o)$ as an independent variable in the Hamilton-Jacobi transformation, i.e.,

$$p_k = \frac{\partial W}{\partial q_k} \quad , \quad q_k(t_o) = \frac{\partial W}{\partial p_k(t_o)}$$

$$H + \frac{\partial W}{\partial t} = 0 \quad .$$

The connection between the two generators W_{qq_o} and W_{qp_o} is provided by

$$W_{q_o p_o} = \sum \tfrac{1}{2} \left\{ q_k(t_o) \quad , \quad p_k(t_o) \right\} \quad ,$$

namely

$$W_{qp_o} = W_{qq_o} + W_{q_o p_o} \quad .$$

For our example,

$$W_{qp_o} = \tfrac{1}{2} \left\{ q, \, p_o \right\} - \frac{p_o^2}{2m} \, t \quad ,$$

which again possesses the form (2.7), with $\alpha = 0$, $\beta = 1$, $\gamma = - \frac{t}{2m}$. Hence

$$[p_o \; q] = \frac{\hbar}{i} \quad ,$$

$$\mathcal{W}(q, \, p_o, \, t) = q \, p_o - \frac{p_o^2}{2m} \, t + \frac{\hbar}{2i} \log \frac{i}{2\pi h} \quad ,$$

and

$$(q' t \,|\, p_o') = e^{\frac{i}{\hbar}\mathcal{W}(q', p', t)} = \left(\frac{i}{2\pi \hbar} \right)^{\frac{1}{2}} e^{\frac{i}{\hbar}\left(q'p' - \frac{p'^2}{2m} t \right)} \quad .$$

Another example is the one dimensional system with

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2 .$$

The equations of motion have the solution

$$q = q_o \cos \omega t + \frac{1}{m\omega} p_o \sin \omega t$$

$$p = - m w q_o \sin \omega t + p_o \cos \omega t ;$$

a linear transformation. On substituting these solutions, the action integral is obtained as

$$W = \left(\frac{p_o^2}{2m} - \frac{m\omega^2}{2} q_o^2\right) \frac{\sin 2\omega t}{2\omega} - \frac{1}{2}\left\{q_o, p_o\right\} \sin^2 \omega t$$

$$= \frac{m\omega}{2} \cot \omega t \left[q^2 - \frac{1}{\cos \omega t} \left\{q, q_o\right\} + q_o^2 \right] .$$

Hence $\alpha = \gamma\, m\omega \cot wt$, $\beta = - m\omega \csc \omega t$, and

$$\left[q_o, q\right] = \frac{i\hbar}{m\omega} \sin \omega t ,$$

$$\mathcal{W} = \frac{m\omega}{2} \cot \omega t \left[q^2 - \frac{2}{\cos \omega t} q q_o + q_o^2\right] + \frac{i\hbar}{2} \log \left(\frac{2\pi\hbar i}{m\omega} \sin \omega t\right)$$

$$(q' t | q_o'') = \left(\frac{m\omega}{2\pi\hbar i} \csc \omega t\right)^{\frac{1}{2}} e^{\frac{i}{\hbar} \frac{m\omega}{2} \cot \omega t \left[q'^2 - \frac{2}{\cos \omega t} q' q'' + q''^2\right]} .$$

<u>Constrained Transformations</u>

A special situation is encountered when the canonical transformation involves one or more relations between the q's and $\bar{q}$'s, so that they are not actually susceptible to independent variations. The simplest example is the identity transformation

$$\bar{q}_k = q_k , \quad \bar{p}_k = p_k$$

where $W(q, \bar{q})$ has the value zero, indicating a relation between the q's and $\bar{q}$'s. Nevertheless, one can treat the q's and $\bar{q}$'s as independent variables, and derive the transformation equations from a suitable W, provided one introduces an intermediate transformation not so handicapped and refrains from eliminating the intermediate variables. Thus, describe the identity transformation as $q \rightarrow p \rightarrow \bar{q}$ for which

$$W = \sum \tfrac{1}{2}\left\{q_k, p_k\right\} - \tfrac{1}{2}\sum\left\{\bar{q}_k, p_k\right\} \quad .$$

We have

$$\delta W = \sum (q_k - \bar{q}_k)\delta p_k + \sum p_k \delta q_k - \sum p_k \delta \bar{q}_k$$

$$= \sum p_k \delta q_k - \sum \bar{p}_k \delta \bar{q}_k$$

from which follows the desired equations.

For the general "point transformation",

$$q_k = q_k(\bar{q}) \quad ,$$

the appropriate Hermitian operator W is

$$W = \sum \tfrac{1}{2}\left\{q_k - q_k(\bar{q}), p_k\right\}$$

since

$$\delta W = \sum (q_k - q_k(\bar{q}))\delta p_k + \sum p_k \delta q_k - \sum \tfrac{1}{2}\left\{\frac{\partial q_k(\bar{q})}{\partial \bar{q}_\gamma}, p_k\right\}\delta \bar{q}_\gamma$$

$$= \sum p_k \delta q_k - \sum \bar{p}_k \delta \bar{q}_k$$

yields the desired relation between the q's and $\bar{q}$'s, and the information

$$\bar{p}_\ell = \sum_h \tfrac{1}{2}\left\{\frac{\partial q_k(\bar{q})}{\partial \bar{q}_\ell}, p_k\right\} .$$

The latter expression can also be written

$$\bar{p}_\ell = \sum p_k \frac{\partial q_k(\bar{q})}{\partial \bar{q}_\ell} + \frac{i\hbar}{2} \sum \frac{\partial \bar{q}_m}{\partial q_k} \frac{\partial}{\partial \bar{q}_\ell} \frac{\partial q_k}{\partial \bar{q}_m}$$

$$= \sum p_k \frac{\partial q_k(\bar{q})}{\partial \bar{q}_\ell} + \frac{i\hbar}{2} \frac{\partial}{\partial \bar{q}_\ell}\left(\log \det \frac{\partial q}{\partial \bar{q}}\right)$$

$$= \sum \frac{\partial q_k(\bar{q})}{\partial \bar{q}_\ell} p_k - \frac{i\hbar}{2} \frac{\partial}{\partial \bar{q}_\ell}\left(\log \det \frac{\partial q}{\partial \bar{q}}\right) .$$

To construct $(q'|\bar{q}'')$ we order δW with respect to q_k and $\bar{q}_k$,

$$\delta W = \sum (q_k \delta p_k - \delta p_k q_k(\bar{q})) + \sum \delta q_k p_k - \sum p_k \frac{\partial q_k(\bar{q})}{\partial \bar{q}_\ell} \delta \bar{q}_\ell$$

$$- \frac{i\hbar}{2} \sum \frac{\partial}{\partial \bar{q}_\ell}\left(\log \det \frac{\partial q}{\partial \bar{q}}\right) \delta \bar{q}_\ell$$

thus obtaining the differential equation

$$\delta(q'|\bar{q}'') = \frac{i}{\hbar} \sum \delta p_k (q_k' - q_k(\bar{q}''))(q'|\bar{q}'') + \sum \delta(q_k' - q_k(\bar{q}'')) \frac{\partial}{\partial q_k'} (q'|\bar{q}'')$$

$$+ \tfrac{1}{2} \delta \left(\log \det \frac{\partial q}{\partial \bar{q}''}\right)(q'|\bar{q}'') .$$

We infer the conditions of constraint on the transformation function

$$\left[q_k' - q_k(\bar{q}'')\right] (q'|\bar{q}'') = 0 ,$$

and a simpler differential equation whose solution in terms of an arbitrary function is fixed by the constraint equations as

$$(q'|\bar{q}'') = (\det \frac{\partial q}{\partial \bar{q}''})^{\frac{1}{2}} \delta(q' - q(\bar{q}'')) \quad .$$

In connection with this example, note the strict requirement that the q's and $\bar{q}$'s be uniquely connected by an everywhere non-singular transformation. Should these conditions be violated, the new variables will not possess all the canonical attributes. We may then speak of a quasi-canonical transformation. A familiar example is the transformation from rectangular to spherical coordinates, where the angle ϕ is only defined mod 2π, and the determinant vanishes at $r = 0$ and at $\vartheta = 0, \pi$. Thus, spherical coordinates are quasi-canonical.

A simple dynamical illustration of a constrained transformation is provided by the one-dimensional system with $H = p^2/2m - Fq$, described in terms of the transformation function $(p't|p''0)$. The equations of motion have the solution

$$p = p_0 + F\,t$$

$$q = q_0 + \frac{p_0}{m}\,t + \frac{F}{2m}\,t^2$$

so that there is a relation between the variables of the transformation function, p and p_0. Now

$$\delta W = -\,q\,\delta p + q_0\,\delta p_0 - H\,\delta t$$

$$= -\,q\,\delta(p - p_0 - Ft) - \tfrac{1}{m}(p_0 t + \tfrac{1}{2}Ft^2)\,\delta p_0 - \tfrac{1}{m}(\tfrac{1}{2}p_0^2 + p_0 Ft + \tfrac{1}{2}F^2t^2)\,\delta t$$

which requires no explicit ordering to write it as δW. We thus obtain the differential equation

$$\delta(p't|p''0) = \delta(p' - p'' - Ft) \frac{\partial}{\partial p'} (p't|p''0)$$

$$- \frac{i}{\hbar} \delta\left(\frac{p''^2}{2m} t + p'' \frac{Ft^2}{2m} + \frac{F^2t^3}{6m}\right) (p't|p''0) \quad ,$$

which is supplemented by the constraint condition

$$(p' - p'' - Ft)(p't|p''0) = 0 \quad .$$

The solution is

$$(p't|p''0) = \delta(p' - p'' - Ft)\, e^{-\frac{i}{\hbar}\left(\frac{p''^2}{2m}t + p''\frac{Ft^2}{2m} + \frac{F^2t^3}{6m}\right)}$$

$$= \delta(p' - p'' - Ft)\, e^{-\frac{i}{\hbar}\frac{1}{6mF}(p'^3 - p''^3)} \quad .$$

On placing $F = 0$, we obtain the transformation function for the system with $H = p^2/2m$:

$$(p't|p''0) = \delta(p' - p'')\, e^{-\frac{i}{\hbar}\frac{p'^2}{2m}t} \quad .$$

Non-Unitary Transformations

Canonical transformations are representable as unitary transformations

$$\bar{q}_h = U q_h U^{-1} \quad , \qquad \bar{p}_h = U p_h U^{-1}$$

in virtue of the identical spectra of all canonical variables. However, for the purpose of preserving the algebraic structure of the

canonical commutation relations, and thereby the canonical equations of motion, it is not necessary that U be a unitary operator. Of course, other features of a canonical transformation will be sacrificed. An example is provided by the point transformation of the previous section. We have

$$\sum p_k \frac{\partial q_k(\bar{q})}{\partial \bar{q}_\chi} = \bar{p}_\chi - \frac{i\hbar}{2}\frac{\partial}{\partial \bar{q}_\chi}\left(\log \det \frac{\partial q}{\partial \bar{q}}\right)$$

$$= \left(\det \frac{\partial q}{\partial \bar{q}}\right)^{-\frac{1}{2}} \bar{p}_\chi \left(\det \frac{\partial q}{\partial \bar{q}}\right)^{\frac{1}{2}} = \hat{p}_\chi \quad .$$

For this canonical, non-unitary transformation

$$U = \left(\det \frac{\partial q}{\partial \bar{q}}\right)^{-\frac{1}{2}}$$

and

$$\hat{q}_\chi = U \bar{q}_\chi U^{-1} = \bar{q}_\chi \quad .$$

Now

$$\Psi(\hat{q}') = U \Psi(\bar{q}') = \Psi(q') \quad , \qquad q' = q(\bar{q}') = q(\hat{q}')$$

and

$$-\hat{p}_\chi \Psi(\hat{q}') = \sum \frac{\partial q_k'}{\partial \bar{q}_\chi'} \frac{\hbar}{i} \frac{\partial}{\partial q_k'} \Psi(q')$$

$$= \frac{\hbar}{i} \frac{\partial}{\partial \hat{q}_\chi'} \Psi(\hat{q}') \quad .$$

However

$$\Psi(\hat{q}')^{+} = \Psi(\bar{q}')^{+}\, U \;(\neq \Psi(\bar{q}')^{+}\, U^{-1})$$

so that the eigenvector orthonormality conditions read

$$(\Phi(\hat{q}')\Psi(\hat{q}'') = \delta(\hat{q}' - \hat{q}'')$$

where

$$\Phi(\hat{q}') = \Psi(\hat{q}')^{+} \det \frac{\partial q}{\partial \hat{q}'} \quad .$$

Hence the dual and Hermitian adjoint eigenvectors are no longer the same. In virtue of the non-Hermitian nature of $\hat{p}_\chi$, it is the dual eigenvector that satisfies

$$\Phi(\hat{q}')\,\hat{p}_\chi = \frac{\hbar}{i}\,\frac{\partial}{\partial \hat{q}'_\chi}\,\Phi(\hat{q}') \quad .$$

This non-unitary transformation corresponds to the familiar procedure of replacing one set of coordinates by another, without transforming the eigenvectors. The determinant of the transformation then enters as a weight factor in all integrals and orthonormality statements.

Non-Hermitian canonical variables are useful in discussing the harmonic oscillator. Thus

$$\bar{q} = a = \left(\frac{m\omega}{2\hbar}\right)^{\frac{1}{2}} \left(q + \frac{i}{m\omega}\,p\right)$$

$$\bar{p} = i\hbar\, a^{+} = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} (p + im\omega\, q)$$

are canonical variables,

$$[a, a^{+}] = 1 \quad ,$$

in terms of which this Hamiltonian can be written

$$H = -i\,\omega\,\tfrac{1}{2}\left\{\bar{q}, \bar{p}\right\} = \hbar\,\omega\,\tfrac{1}{2}\left\{a, a^{+}\right\} \quad .$$

The canonical equations of motion,

$$\frac{da}{dt} = \frac{1}{i\hbar}\,\frac{\partial H}{\partial a^{+}} = -i\,\omega\,a$$

$$\frac{da^{+}}{dt} = -\frac{1}{i\hbar}\,\frac{\partial H}{\partial a^{+}} = i\,\omega\,a^{+} \quad ,$$

are solved by

$$a = a_{o}\,e^{-i\omega t} \quad , \quad a^{+} = a_{o}^{+}\,e^{i\omega t} \quad .$$

A convenient Hamilton-Jacobi transformation employs a_{o} and a^{+} as independent variables. Thus

$$\delta W = -i\,\hbar\,a\,\delta a^{+} - i\,\hbar\,a_{o}^{+}\,\delta\,a_{o} - H\,\delta\,t$$

whence

$$\delta W = -i\,\hbar\,\delta\,a^{+}\,a_{o}\,e^{-i\omega t} - i\,\hbar\,a^{+}\delta\,a_{o}\,e^{-i\omega t} - \hbar\,\omega(a^{+}\,a_{o}\,e^{-i\omega t} + \tfrac{1}{2})\,\delta\,t$$

and

$$W(a^{+}, a_{o}, t) = -i\,\hbar\,a^{+}\,a_{o}\,e^{-i\omega t} - \tfrac{1}{2}\,\hbar\,\omega\,t + \text{Const.}$$

If we introduce eigenvectors of a^{+} and a_{o}, in a purely heuristic manner, we can express the latter result as

$$(a^{+\prime}\ t\,|a''0) = e^{i/\hbar\,W(a^{+\prime}a''t)}$$

$$= e^{-\frac{i}{2}\omega t}\,e^{a^{+\prime}a''e^{-i\omega t}}$$

choosing the multiplicative constant to be unity. In particular, for $t = 0$,

$$(a^{+'}|a'') = e^{a^{+'}a''} = e^{-\frac{i}{\hbar}p'q''} .$$

The transformation functions connecting the eigenvectors of a and a^+ with the eigenvectors of q can be obtained from the theory of the general linear transformation. We find

$$(q'|a') = C\, e^{-\frac{1}{2}[\lambda q'^2 + a'^2 - 2\sqrt{2\lambda}\, q'a']}$$

$$(a^{+'}|a') = C' e^{-\frac{1}{2}[\lambda q'^2 + a^{+'2} - 2\sqrt{2\lambda}\, q'a^{+'}]}$$

$$(a'|q') = C''\, e^{+\frac{1}{2}[\lambda q'^2 + a'^2 - 2\sqrt{2\lambda}\, q'a']}$$

$$(q'|a^{+'}) = C'''\, e^{+\frac{1}{2}[\lambda q'^2 + a^{+'2} - 2\sqrt{2\lambda}\, q'\, a^{+'}]}$$

where $\lambda = m\omega/\hbar$.

Accordingly $(q'|a')^*$ is not equal to $(a'|q')$, but rather can be identified with $(a^{+'}|q')$, provided the eigenvalues of a and a^+ are complex numbers related by

$$a^{+'} = (a')^* .$$

The constant $C' = C^*$ can then be fixed from the requirement

$$(a^{+'}|a'') = \int (a^{+'}|q')\, d\, q'(q'|a'')$$

$$= |C|^2 \left(\frac{\pi}{\lambda}\right)^{\frac{1}{2}} e^{a^{+'}a''} .$$

This is satisfied with

$$C = C' = \left(\frac{\lambda}{\pi}\right)^{1/4} .$$

On the other hand, note that

$$(a'|a^{+''}) = \int (a'|q')d\,q'(q'|a^{+''})$$

does not exist.

<u>Infinitesimal Canonical Transformations</u>

An infinitesimal canonical transformation

$$\bar{q}_k = q_k - \delta q_k$$

$$\bar{p}_k = p_k - \delta p_k$$

can be generated by a W which differs infinitesimally from the generator of the identity transformation,

$$W = \sum \frac{1}{2}\left\{q_k - \bar{q}_k,\ p_k\right\} - F(\bar{q}, p, t) .$$

Whether one writes $\bar{q}$ or q in the infinitesimal operator F is immaterial for its value, but is relevant in the derivation of the canonical transformation. Now

$$\delta W = \sum p_k \delta q_k - \sum \left(p_k + \frac{\partial F(q,p,t)}{\partial q_k}\right) \delta \bar{q}_k$$

$$+ \sum \left(\delta q_k - \frac{\partial F}{\partial p_k}\right) \delta p_k - \frac{\partial F}{\partial t}\ \delta t$$

$$= \sum p_k \delta q_k - \sum \bar{p}_k \delta \bar{q}_k - (H - \bar{H}) \delta t$$

whence

$$\delta q_k = \frac{\partial F(qpt)}{\partial p_k} \quad , \quad \delta p_k = - \frac{\partial F(qpt)}{\partial q_k}$$

$$H(qpt) - \bar{H}(\bar{q}\bar{p}t) = \frac{\partial}{\partial t} F(qpt)$$

characterize a general infinitesimal canonical transformation. We can also write

$$\delta q_k = \frac{1}{i\hbar} [q_k, F] \quad , \quad \delta p_k = \frac{1}{i\hbar} [p_k, F]$$

which shows that F is the infinitesimal Hermitian generator of the equivalent unitary transformation.

The effect of the transformation on an arbitrary function G(qpt) can be computed directly,

$$\begin{aligned} \delta G &= G(qpt) - G(\bar{q}\bar{p}t) \\ &= G(qpt) - G(q - \frac{\partial F}{\partial p} \ , \ p + \frac{\partial F}{\partial q} , t) \ , \end{aligned}$$

or

$$\partial G = \sum \left(\frac{\partial G}{\partial q_k} \frac{\partial F}{\partial p_k} - \frac{\partial G}{\partial p_k} \frac{\partial F}{\partial q_k} \right) \equiv (G, F) \ ,$$

which defines the Poisson bracket of two operators. The notation is symbolic in that $\frac{\partial F}{\partial p_k}$, say, occurs in definite places in the structure of G. We also have

$$\delta G = \frac{1}{i\hbar} [G, F]$$

which expresses the Poisson bracket in terms of the commutator

$$(G, F) = \frac{1}{i\hbar}[G, F] \quad .$$

From this connection it follows that

$$(G, F) = -(F, G) \quad ,$$

although this is not quite evident from the definition.

We obtain from these results

$$\bar{H}(\bar{q}\bar{p}t) = \bar{H}(qpt) + (F, H)$$

$$= H(qpt) - \frac{\partial}{\partial t} F$$

or

$$\bar{H}(qpt) = H(qpt) - \frac{\partial}{\partial t} F - (F, H)$$

$$= H(qpt) - \frac{dF}{dt} \quad ,$$

in virtue of the Poisson bracket form of the general equations of motion. This implies that the generator of any transformation that leaves the <u>form</u> of the Hamiltonian unchanged is a constant of the motion.

<u>Parameterized Transformations</u>

Let us suppose that the infinitesimal transformation is that associated with an infinitesimal change $- d\tau_r$ of certain parameters τ_r, so that F has the form

$$F = - \sum_r F_{(r)}\, d\tau_r$$

and

$$\delta q_k = \sum \frac{dq_k}{d\tau_r} d\tau_r = dq_k \quad .$$

Thus

$$W_{d\tau} = \sum \tfrac{1}{2} \left\{ p_k, dq_k \right\} + \sum F_{(r)} \, d\tau_r$$

and

$$\delta(q'\tau | q''\tau - d\tau) = \frac{i}{\hbar} (q'\tau | \delta W_{d\tau} | q''\tau - d\tau) \quad .$$

A finite canonical transformation, $(q'\tau_1 | q''\tau_2)$, can now be characterized by adding the generators of an infinite sequence of infinitesimal transformations,

$$W_{12} = \int_{\tau_2}^{\tau_1} \left[\sum_k \tfrac{1}{2} \left\{ p_k, dq_k \right\} + \sum_r F_{(r)} \, d\tau_r \right] \quad .$$

In particular, with the single parameter $\tau = t$, and $F = -H$, we regain the original action principle.

We compute δW_{12},

$$\delta W_{12} = \int d\left[\sum_k p_k \, \delta q_k + \sum_r F_{(r)} \, \delta\tau_r \right]$$

$$+ \int \left[\sum_k (\delta p_k dq_k - d\, p_k \delta q_k) + \sum_r (\delta F_{(r)} d\tau_r - dF_{(r)} \, \delta\tau_r) \right] \quad .$$

In order that a finite transformation be generated, the coefficients of the intermediate δq_k and δp_k must be zero. This yields the equations of motion

$$-\frac{dq_k}{d\tau_r} = \frac{\partial F_{(r)}}{\partial p_k} \quad , \quad \frac{dp_k}{d\tau_r} = \frac{\partial F_{(r)}}{\partial q_k} \quad ,$$

which repeat the original assertion that $F_{(r)}\, d\tau_r$ is the generator of the infinitesimal change $d\tau_r$ in τ_r. Hence

$$\delta W_{12} = F_1 - F_2 - \int \sum \left(\frac{dF_{(r)}}{d\tau_s} - \frac{\partial F_{(s)}}{\partial \tau_r} \right) \delta\tau_r \, d\tau_s$$

where

$$F = \sum p_k \, \delta q_k + \sum F_{(r)} \, \delta \tau_r \quad .$$

The last term of δW_r allows for the possibility that the transformation function may depend upon the integration path of the τ variables. Now, according to the significance of $F_{(s)}\; d\tau_{(s)}$, we have for any operator G,

$$\frac{1}{i\hbar}\left[G, F_{(s)}\, d\tau_s\right] = \delta_s G = -\left(\frac{dG}{d\tau_s} - \frac{\partial G}{\partial \tau_s} \right) d\tau_s$$

or

$$\frac{dG}{d\tau_s} = \frac{\partial G}{\partial \tau_s} + (F_{(s)}, G) \quad .$$

In particular,

$$\frac{dF_{(r)}}{d\tau_s} = \frac{\partial F_{(r)}}{\partial \tau_s} + (F_{(s)}, F_{(r)}) \quad .$$

Hence

$$A_{rs} = \frac{dF_{(r)}}{d\tau_s} - \frac{\partial F_{(s)}}{d\tau_r} = \frac{\partial F_{(r)}}{\partial \tau_s} - \frac{\partial F_{(s)}}{\partial \tau_r} + (F_{(s)}, F_{(r)})$$

is anti-symmetrical with respect to the indices r and s. The change in the transformation function produced by an alteration of the integration path is thus given by

$$\delta(q'\tau_1|q''\tau_2) = -\frac{i}{\hbar}(q'\tau_1|\int_{\tau_2}^{\tau_1} A_{rs}\,\tfrac{1}{2}(\delta\tau_r\, d\tau_s - \delta\tau_s\, d\tau_r)|q''\tau_2) \quad .$$

The simplest possibility is $A_{rs} = 0$; the transformation function is independent of the integration path. Second in the hierarchy of complications is $A_{rs} = a_{rs}(\tau)$, a numerical function. Here the transformation function depends upon the path only to the extent of a phase constant which is independent of q' and q'', etc. We shall be content with the first situation - independence of path. In particular if the $F_{(r)}$ do not involve the parameters, they must satisfy

$$[F_{(r)}, F_{(s)}] = 0 \quad .$$

Now suppose that the $F_{(r)}$ form a complete set of commuting operators so that we may introduce the eigenvectors $\Psi(F'\tau)$. The transformation function $(F'\tau_1|F''\tau_2)$ is determined by

$$\frac{\partial}{\partial\tau_{1r}}(F'\tau_1|F''\tau_2) = \frac{i}{\hbar}(F'\tau_1|F_{(r)}|F''\tau_2) = \frac{i}{\hbar}F'_r(F'\tau_1|F''\tau_2)$$

in conjunction with the boundary condition

$$(F'\tau_2|F''\tau_2) = \delta(F', F'') \quad ,$$

(assuming discrete eigenvalues). Hence

$$(F'\tau_1|F''\tau_2) = e^{\frac{i}{\hbar}\Sigma F'_r\tau_r}\,\delta(F',F'') \quad , \quad \tau = \tau_1 - \tau_2 \quad .$$

But the canonical transformation function $(q'\tau_1|q''\tau_2)$ can be written

$$(q'\tau_1|q''\tau_2) = \sum (q'\tau_1|F'\tau_1)(F'\tau_1|F''\tau_2)(F''\tau_2|q''\tau_2)$$

$$= \sum_{F'} (q'|F')\, e^{\frac{i}{\hbar}\Sigma F'_r\tau_2} (F'|q'') \quad ,$$

or, with a notational change

$$(q'\tau_1|q''\tau_2) = \sum_{r=1} \psi_{F'}(q')\, e^{\frac{i}{\hbar}\Sigma F'_r\tau_r}\, \psi_{F'}(q'')^* \quad .$$

Accordingly if one can construct the transformation function describing the finite canonical transformation generated by the $F_{(r)}$, the expansion of that transformation function in exponentials of the τ_r will yield all the eigenvalues and eigenfunctions of the arbitrary complete set of commuting operators.

We illustrate this with two transformation functions already obtained for a system of one degree of freedom and $\tau = t$, $F = -H$. For the harmonic oscillator,

$$(a^{+\prime}t|a''0) = e^{-\frac{i}{2}wt}\, e^{a^{+\prime}a''e^{-iwt}}$$

$$= \sum_{m=o}^{\infty} \frac{(a^{+\prime})^n}{\sqrt{n!}}\, e^{-\frac{i}{\hbar}(n+\frac{1}{2})\hbar wt}\, \frac{(a'')^n}{\sqrt{n!}} \quad .$$

so that the eigenvalues of the Hamiltonian are

$$E_n = (n + \tfrac{1}{2})\,\hbar w \quad , \qquad h = 0, 1, \ldots$$

and

$$(a^{+\prime}|n) = \frac{(a^{+\prime})^n}{\sqrt{n!}}$$

$$(n|a') = \frac{a'^n}{\sqrt{n!}}$$

which satisfy

$$(a^{+\prime}|n) = (n|a')^* \quad .$$

The eigenfunctions $(q'|n) = \psi_n(q')$ can then be constructed from the transformation function

$$(q'|a') = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}q'^2 - \frac{1}{2}a'^2 + \sqrt{\frac{2m\omega}{\hbar}}\,q'a'}$$

$$= \sum \psi_n(q')\,\frac{a'^n}{\sqrt{n!}} \quad ,$$

which is, essentially, the well-known generating function of the Hermite polynomials.

For the particle exposed to a constant force, we found

$$(p't|p''0) = \delta(p' - p'' - F\tau)\; e^{-\frac{i}{\hbar}\frac{1}{6mF}(p'^3 - p''^3)} \quad .$$

If one inserts the integral representation of the delta function,

$$\delta(p' - p'' - F\tau) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \frac{dE}{F}\, e^{\frac{i}{\hbar}\frac{E}{F}(p' - p'' - F\tau)}$$

one obtains

$$(p't|p''0) = \int_{-\infty}^{\infty} (p'|E)dE\, e^{-\frac{i}{\hbar}Et}(E|p'')$$

where

$$(p'|E) = (2\pi\hbar F)^{-\frac{1}{2}}\, e^{\frac{i}{\hbar}\frac{1}{F}(Ep' - \frac{p'^3}{6m})} \quad ;$$

for this problem the Hamiltonian has a spectrum ranging continuously from $-\infty$ to ∞. Hence H is a canonical variable. In fact, with

$$\bar{p} = H = \frac{p^2}{2m} - Fq \quad ,$$

$$\bar{q} = \frac{1}{F}\, p \quad ,$$

we have

$$(\bar{q}, \bar{p}) = 1 \quad .$$

The transformation function $(p'|\bar{p}'')$ can now be constructed from

$$\delta W = -q\,\delta p + \bar{q}\,\delta\bar{p} = \frac{1}{F}(\bar{p} - \frac{p^2}{2m})\,\delta p + \frac{1}{F}\,p\,\delta\bar{p} \quad .$$

We get

$$(p, \bar{p}) = \frac{1}{F}\left(p\,\bar{p} - \frac{p^3}{6m}\right) + \text{Const} \quad ,$$

and, writing $\bar{p}' = E$,

$$(p'|E) = C\, e^{\frac{i}{\hbar}\frac{1}{F}(p'E - \frac{p'^3}{6m})} \quad .$$

But

$$\int (E|p')dp'(p'|E') = |C|^2 \int_{-\infty}^{\infty} e^{\frac{i}{\hbar}\frac{p'}{F}(E-E')}\,dp' = |C|^2 2\pi\hbar F\,\delta(E - E')$$

whence

$$C = (2\pi\hbar F)^{-\frac{1}{2}} \quad .$$

Notice that the transformed function $(p'|E)$ has a singularity at $F = 0$, corresponding to the fact that the Hamiltonian $H = \frac{p}{2m}$ is not a canonical variable.

Green's Functions

A general method for constructing the transformation function $(q'\tau|q''0)$ is based upon the differential equation

$$\frac{\hbar}{i}\frac{\partial}{\partial\tau_r}(q'\tau|q''0) = (q'\tau|F_{(r)}(q\ p)|q''0)$$

$$= F_{(r)}(q', \frac{\hbar}{i}\frac{\partial}{\partial q'})(q'\tau|q''0)$$

in which the use of the differential operator $F_{(r)}(q', \frac{\hbar}{i}\frac{\partial}{\partial q'})$ is only illustrative; integral operators can also occur. These equations are to be supplemented by the boundary condition

$$(q'0|q''0) = \delta(q' - q'') \quad .$$

In particular,

$$i\hbar\frac{\partial}{\partial t}(q't|q''0) = H(q', \frac{\hbar}{i}\frac{\partial}{\partial q'})(q't|q''0)(q'0|q''0)$$

$$(q'0|q''0) = \delta(q' - q'') \quad .$$

Turning to the simpler situation of a single parameter, we note that the boundary condition can be incorporated into the differential equations by defining the discontinuous Green's function:

$$G(q' q'', t) = \frac{1}{i\hbar} (q't | q''0) \quad , \quad t > 0$$

$$= 0 \qquad\qquad , \quad t < 0 \; .$$

Indeed,

$$\left[i \hbar \frac{\partial}{\partial t} - H \left(q', \frac{\hbar}{i} \frac{\partial}{\partial q'} \right) \right] G(q' q'' t) = \delta(t) \delta(q' - q'') \quad ,$$

and we now seek the solution of this inhomogeneous equation which vanishes for negative τ. If, as we have tacitly assumed, the Hamiltonian is time-independent, the Green's function equation can be given another, convenient form in terms of the Fourier transform

$$G(q'q'', E) = \int_{-\infty}^{\infty} dt \, e^{\frac{i}{\hbar}Et} \, G(q', q'', t) \quad , \qquad I m E > 0$$

namely

$$\left[E - H(q', \frac{\hbar}{i} \frac{\partial}{\partial q'}) \right] G(q', q'', E) = \delta(q' - q'') \quad .$$

We now desire a solution which, as a function of the complex variable E, is regular in the upper-half plane. Since

$$G(q'q'', E) = \int_0^{\infty} dt \, e^{\frac{i}{\hbar}Et} \frac{1}{i\hbar} \sum_{E'\gamma'} \psi_{E'\gamma'}(q') \, e^{-\frac{i}{\hbar}E't} \psi_{E'\gamma'}(q'')^*$$

$$= \sum_{E'\gamma'} \frac{\psi_{E'\gamma'}(q') \, \psi_{E'\gamma'}(q'')^{-*}}{E - E'} \quad ,$$

here γ, in conjunction with the Hamiltonian forms a complete set, we see that the poles of $G(q'q'' E)$ as a function of E are the eigenvalues E', and the residues yield the eigenfunctions.

For the general problem of n parameters τ_r, we define

$$G(q'q''\tau) = \left(\frac{i}{\hbar}\right)^n (q'\tau|q''0) \quad , \quad \tau_r > 0$$

$$= 0 \qquad\qquad , \text{ any } \tau_r < 0 \ .$$

Hence

$$\left[\frac{\hbar}{i}\frac{\partial}{\partial\tau_1} - F_{(1)}\left(q', \frac{\hbar}{2}\frac{\partial}{\partial q'}\right)\right] G(q\ q', \tau) = \delta(\tau_1)\left(\frac{i}{\hbar}\right)^{h-1}(q'\tau|q''0)\Big|_{\tau_1=0}$$

and finally

$$\prod_{r=1}^{n}\left[\frac{\hbar}{i}\frac{\partial}{\partial\tau_r} - F_{(r)}\left(q', \frac{\hbar}{i}\frac{\partial}{\partial q'}\right)\right] G(q\ q', \tau) = \delta(\tau)\,\delta(q' - q'') \ .$$

The Fourier transform

$$G(q'\ q'', f) = \int d\tau\, e^{-\frac{i}{\hbar}\sum_r f_r\tau_t} G(q'q'', \tau) \quad , \quad \mathrm{Im}\, f_r < 0$$

obeys

$$\prod_{r=1}^{n}\left[\left(f_r - F_{(r)}(q', \frac{\hbar}{2}\frac{\partial}{\partial q'}\right)\right] G(q'\ q'', f) = \delta(q' - q'')$$

and

$$G(q', q'', f) = \sum_{F'}{}' \frac{\psi_{F'}(q')\,\psi_{F'}(q'')^*}{\prod_r (f_r - F_r')} \ .$$

The Asymptotic Spectrum

If the operations $F_{(r)}$ are polynomials in the p_k, one can easily construct the transformation function $(q'\tau + d\tau|p'\tau)$. The appropriate W is:

$$W = \Sigma \tfrac{1}{2}\left\{q_k(\tau + d\tau) - q_k(\tau) \quad , \quad p_k(\tau)\right\} + \Sigma F_{(r)}\, d\tau_r$$

$$+ \Sigma \tfrac{1}{2}\left\{q_k(\tau) \quad , \quad p_k(\tau)\right\}$$

$$= \Sigma \tfrac{1}{2}\left\{q_k(\tau + d\tau) \quad , \quad p_k(\tau)\right\} + \Sigma F_{(r)}\, d\tau \quad .$$

We compute δW and order it into $\delta \mathcal{W}$, which must be explicitly possible if the $F_{(r)}$ are polynomials in the p_k. Thus,

$$\mathcal{W} = \Sigma\, q_k(\tau + d\tau)\, p_k(\tau) + \Sigma\, \mathcal{F}_r\, (q(\tau + d\tau), p(\tau))\, d\tau_r$$

and

$$(q'\tau + d\tau|p'\tau) = \left(\frac{i}{2\pi\hbar}\right)^{n/2} e^{\frac{i}{\hbar}[\sum_k q'_k p'_k + \sum_r \mathcal{F}_r(q',p')d\tau_r]} \quad .$$

With the aid of this transformation function, one obtains

$$(q'\tau + d\tau|q''\tau) = \int (q'\tau + d\tau|p'\tau)d\, p'(p'|q'')$$

$$= \frac{1}{(2\pi\hbar)^n}\int d\, p'\; e^{\frac{i}{\hbar}[\Sigma(q'-q'')_k p'_k + \Sigma \mathcal{F}_r(q'p')d\tau_r]} \quad .$$

A general application of this formula involves the computation of the quantity yielding all the eigenvalues,

$$\int dq'(q'\tau_1|q'\tau_2) = \int d\,q' \sum (q'|F')\, e^{\frac{i}{\hbar}\Sigma F'_r\tau_r} (F'|q')$$

$$= \sum_{F'} e^{\frac{i}{\hbar}\sum_r F'_r\tau_r} ,$$

in the limit of infinitesimal $\tau_1 - \tau_2$. We get

$$\int dq'(q'\tau + d\,\tau|q'\tau) = \int \frac{dq'dp'}{(2\pi\hbar)^n}\, e^{\frac{i}{\hbar}\sum_r \mathcal{F}_r(q'p')d\tau_r}$$

$$= \sum_{F'} e^{\frac{i}{\hbar}\sum_r F'_r d\tau_r} ,$$

If we write

$$\int_{F' \leq \mathcal{F} < F'+dF'} \frac{dq'dp'}{(2\pi\hbar)^n} = \rho(F')dF' ,$$

this result becomes

$$\sum_{F'} e^{\frac{i}{\hbar}\Sigma F'_r d\tau_r} = \int \rho(F')\, d\,F'\, e^{\frac{i}{\hbar}\Sigma F'_r d\tau_r} .$$

Evidently for infinitesimal $d\tau_r$, the sum is dominated by the dense, essentially continuous part of the spectrum and $\rho(F')\,dF'$ is the number of states in the eigenvalue range dF'. This can be expressed by the familiar rule that there is one state per volume $(2\pi\hbar)^n$ of phase space.

December 19, 1952

THE NATIONAL BUREAU OF STANDARDS

Functions and Activities

The functions of the National Bureau of Standards are set forth in the Act of Congress, March 3, 1901, as amended by Congress in Public Law 619, 1950. These include the development and maintenance of the national standards of measurement and the provision of means and methods for making measurements consistent with these standards; the determination of physical constants and properties of materials; the development of methods and instruments for testing materials, devices, and structures; advisory services to Government Agencies on scientific and technical problems; invention and development of devices to serve special needs of the Government; and the development of standard practices, codes, and specifications. The work includes basic and applied research, development, engineering, instrumentation, testing, evaluation, calibration services and various consultation and information services. A major portion of the Bureau's work is performed for other Government Agencies, particularly the Department of Defense and the Atomic Energy Commission. The scope of activities is suggested by the listing of divisions and sections on the inside of the front cover.

Reports and Publications

The results of the Bureau's work take the form of either actual equipment and devices or published papers and reports. Reports are issued to the sponsoring agency of a particular project or program. Published papers appear either in the Bureau's own series of publications or in the journals of professional and scientific societies. The Bureau itself publishes three monthly periodicals, available from the Government Printing Office: The Journal of Research, which presents complete papers reporting technical investigations; the Technical News Bulletin, which presents summary and preliminary reports on work in progress; and Basic Radio Propagation Predictions, which provides data for determining the best frequencies to use for radio communications throughout the world. There are also five series of nonperiodical publications: The Applied Mathematics Series, Circulars, Handbooks, Building Materials and Structures Reports, and Miscellaneous Publications.

Information on the Bureau's publications can be found in NBS Circular 460, Publications of the National Bureau of Standards ($1.00). Information on calibration services and fees can be found in NBS Circular 483, Testing by the National Bureau of Standards (25 cents). Both are available from the Government Printing Office. Inquiries regarding the Bureau's reports and publications should be addressed to the Office of Scientific Publications, National Bureau of Standards, Washington 25, D. C.

NBS