II

THE SPHERICAL SYMMETRY OF ATOMS

An atom or an ion, whose nucleus is considered as a fixed center of force O, possesses two kinds of symmetry properties: (1) the laws governing it are spherically symmetric, i.e., invariant under an arbitrary rotation about O; (2) it is invariant under permutation of its f electrons. The first type of symmetry is described by the continuous group[1] γ of orthogonal transformations of the spacial coordinates x, y, z, and the second by the finite symmetric group of order $f!$ which consists of all permutations of f things. This accounts for the importance of these two groups in physics. It is my intention to give a general idea of what the first kind of symmetry means for quantum physics. But before taking up these applications of group theory I find it desirable to describe the general foundations of quantum mechanics as briefly as possible.

Let the physical system P under consideration be, as I said before, an atom or an ion consisting of a fixed nucleus in O and f electrons revolving about it. I employ Cartesian coordinates x, y, z with origin in O as the coordinates of the three-dimensional physical space. For the mathematical representation of the state of P we need (in addition to the actual space) an abstract system space which has in general an infinity of dimensions: it is to be a *unitary vector space*. What does that mean? In an n-dimensional Euclidean

[1] For a more extensive treatment of groups see H. Weyl, *Gruppentheorie und Quantenmechanik*, Leipzig, 1928. This book is hereafter referred to as GQ.

vector space each vector $\mathfrak{x}$ is described with respect to a Cartesian or normal coordinate system by its n components $x_1, x_2, \cdots, x_n$. The square of the length of $\mathfrak{x}$ is

$$\mathfrak{x}^2 = x_1^2 + x_2^2 + \cdots + x_n^2. \tag{1}$$

All Cartesian coordinate systems are equally admissible; they are transformed into each other by *orthogonal transformations*, i.e., linear homogeneous transformations which leave the quadratic form (1) invariant. But when the components x_i are allowed to take arbitrary complex values instead of real ones, as is the case in quantum physics, the form (1) loses its positive definite character and must be replaced by

$$\mathfrak{x}^2 = \bar{x}_1 x_1 + \bar{x}_2 x_2 + \cdots + \bar{x}_n x_n \tag{2}$$

where $\bar{x}_i$ is the conjugate complex of x_i. We then speak of unitary instead of Euclidean geometry; linear transformations which leave $\bar{x}_1 x_1 + \cdots + \bar{x}_n x_n$ invariant are called unitary transformations. The scalar product $(\mathfrak{x}\ \mathfrak{y})$ of two vectors $\mathfrak{x}$ and $\mathfrak{y}$ in unitary geometry is defined by

$$(\mathfrak{x}\ \mathfrak{y}) = \bar{x}_1 y_1 + \cdots + \bar{x}_n y_n.$$

The first general principle in the construction of the mathematical skeleton[1] of quantum theory is this:

I. *There is associated with the physical system P a unitary system space* $\mathfrak{R}$; *every state of the system is represented by a vector in* $\mathfrak{R}$. In Schrödinger's wave theory of a single particle this space $\mathfrak{R}$ consists of all functions $\psi\ (x\ y\ z)$ of the coordinates $x\ y\ z$ of the particle for which the integral of $\bar{\psi}\psi$ has a finite value. They form a vector space (of an infinity of dimensions) because these functions allow addition and multiplication with arbitrary complex numbers. The integral just mentioned replaces the sum (2). The undulatory character of physical phenomena, the fact that they show *interference*, i.e., linear superposition with arbitrary shifts

[1] See GQ, §14.

of phase, means that we are dealing with vectors in a complex vector space which are capable of addition and multiplication by complex numbers. It is unitary because there exists something like *intensity*.

A linear transformation

$$x_i' = \Sigma_k \, l_{ik} x_k$$

can be interpreted as an *operator* L which carries the arbitrary vector $\mathfrak{x} = (x_i)$ over into $\mathfrak{x}' = (x_i')$; the linear character of such an operator is described by the functional equations

$$(\mathfrak{x} + \mathfrak{y})' = \mathfrak{x}' + \mathfrak{y}'; \quad (a \cdot \mathfrak{x})' = a \cdot \mathfrak{x}'$$

$L = \|l_{ik}\|$ is the coefficient matrix of L in the chosen normal coordinate system. If we go over to a new normal coordinate system by means of the unitary transformation U the same operator L is expressed by another matrix $L' = \|l'_{ik}\|$ instead of L, namely

$$L' = ULU^{-1}.$$

L is itself unitary if it leaves the square of the length of an arbitrary vector invariant: $\mathfrak{x}'^2 = \mathfrak{x}^2$. L is an Hermitian operator if the scalar product $(\mathfrak{x} \cdot L\mathfrak{y})$ is conjugate complex to the scalar procuct $(\mathfrak{y} \cdot L\mathfrak{x})$; the matrix L then fulfills the condition of symmetry $l_{ki} = \bar{l}_{ik}$. The scalar product

$$(\mathfrak{x} \cdot L\mathfrak{x}) = \Sigma l_{ik} \bar{x}_i x_k$$

is called an Hermitian form.[1]

The main theorem on Hermitian forms is the theorem concerning the existence of principal axes, which is so familiar to you in the two- and three-dimensional Euclidean geometry, where ellipses and ellipsoids appear in place of Hermitian forms. One can always find a normal coordinate system $\mathfrak{e}_i$ in which the given Hermitian form L reduces to

$$\Sigma_i \, l_i \, \bar{x}_i \, x_i$$

or in terms of which the Hermitian operator is expressed by the simple equation $x_i' = l_i x_i$. $\mathfrak{e}_i$ are the characteristic vectors

[1] GQ, p. 17.

("Eigenvektoren" in German) and l_i the corresponding characteristic numbers ("Eigenwerte").

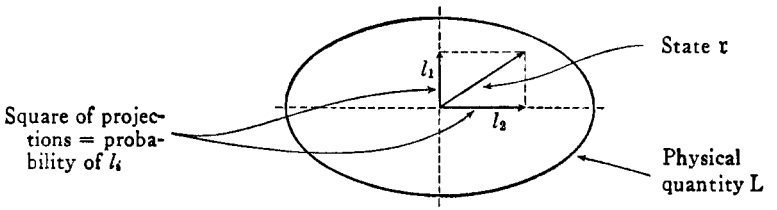
I can express the second and third general principles of quantum theory in terms of these notions. The general question of quantum theory is this: What are the possible values of a given physical quantity L, and what is the probability that it will assume these values when the system is in a given state $\mathfrak{x}$? Before we can answer this question we must know how the state of our physical system and how any quantity L of P can be described mathematically. Principle I takes care of the description of the state $\mathfrak{x}$, and Principle II asserts that:

II. *Each physical quantity L of P is represented by a certain Hermitian operator L in system space* $\mathfrak{R}$.[1]

And on the basis of this mathematical scheme the answer to the general physical question is:

III. *The possible values of a physical quantity L are the characteristic values* l_i *of the Hermitian form L which represents it; the relative probability that it will assume the value* l_i *in the state* $\mathfrak{x}$ *is given by the number* $\bar{x}_i x_i$, *i.e., the square of the absolute value of the projection of* $\mathfrak{x}$ *along the i-th principal axis.*[2]

The situation is the following—*cum grano salis!* (The diagram has been drawn in two instead of an infinite number of dimensions.)



The quantity under consideration will only assume a

[1] GQ, §14. [2] GQ, §5.

value with certainty if $\mathfrak{x}$ falls along one of the principal axes.

In Schrödinger's theory[1] of a single particle the coordinate x is represented by the linear Hermitian operator which carries ψ into $x\psi$ (multiplication by x). This operator $\psi \to x\psi$ is already referred to principal axes; Schrödinger employs that coordinate system in system space in which the operators which represent the coordinates of the electron are referred to principal axes. The probability that the coordinates $x\ y\ z$ of the electron are within a volume V is given by the integral of $\bar{\psi}\psi$ over V, in agreement with our general probability principle III.

The components p_x, p_y, p_z of momentum are represented by the Hermitian operators

$$p_x : \psi \to \frac{h}{2\pi i}\frac{d}{dx}\psi; \cdots$$

in Schrödinger's theory. h is Planck's constant; I shall henceforth employ units which are so chosen that $h/2\pi$ becomes equal to 1.

The fourth principle is the *dynamical law*[2] which asserts that:

IV. *The state* $\mathfrak{x}$ *of the system goes over into a new state* $\mathfrak{x}+d\mathfrak{x}$ *after lapse of time* dt *which arises from* $\mathfrak{x}$ *by an infinitesimal unitary operator*

$$d\mathfrak{x} = \frac{dt}{i} H\mathfrak{x} \quad \text{or} \quad \frac{d\mathfrak{x}}{dt} = \frac{1}{i} H\mathfrak{x}.$$

If I write an arbitrary infinitesimal unitary operator in this form it can be readily shown that H is an Hermitian operator. The quantity represented by H is called *energy*.

I now come back to my proper subject. In addition to the *real* process which carries the state $\mathfrak{x}$ of our physical system

[1] GQ, §10.

[2] GQ, §15.

P at time t over into the new state $\mathfrak{x}'$ at a later time t', I consider a *virtual* process: I rotate P about the origin O by the rotation s; by this process the arbitrary state $\mathfrak{x}$ of P goes over into a new state $\mathfrak{x}'$. Since everything which is physically significant must remain unchanged and since the system space of the vector $\mathfrak{x}$ is unitary, the transition $\mathfrak{x}\to\mathfrak{x}'$ must be a linear unitary operator $U(s)$, dependent on s, in the system space. I say briefly that $U(s)$ is *induced* in the system space by s. All such rotations s form the group of rotations of orthogonal transformations in our 3-dimensional Euclidean space. The correspondence $U: s\to U(s)$ must obey the following law

$$U(t)\,U(s) = U(ts):$$

To the composition of rotations s, t corresponds the composition of the induced operations U in system space. The mathematician calls such a correspondence a *representation*[1] of the rotation group.

The transition $t\to t'$ occurring in real physical time can be generated by the infinitesimal transition $t\to t+dt$, the dynamical law giving the induced infinitesimal unitary operator in system space: $d\mathfrak{x} = \frac{dt}{i} H\mathfrak{x}$. In the same way we may generate the group of rotations by the infinitesimal rotations about the x-, y-, and z-axes. The infinitesimal rotation about the z-axis is given by

$$\delta x = -y, \quad \delta y = x, \quad \delta z = 0. \tag{3}$$

I have purposely written no infinitesimal constant factor ϵ on the right hand side of these equations; you may interpret the differential symbol δ as differentiation $\frac{d}{d\tau}$ with respect to a fictitious or virtual time τ. Let the infinitesimal unitary

[1] GQ, §24.

operator induced in system space by this infinitesimal rotation be

$$\delta\mathfrak{x} = -iM_x\mathfrak{x}.$$

M_x, M_y, M_z are then Hermitian operators; I call them, or rather the physical quantities represented by them the components of angular momentum M. Angular momentum has therefore the same significance for the virtual alteration of $\mathfrak{x}$ by rotation as the energy has for the real alteration of the system P in time.

It can be easily deduced from the dynamical law that a physical quantity A is constant in time when its representing Hermitian operator commutes with H : $HA = AH$. That it is constant here means that the probabilities with which the quantity assumes its different values do not change in time. Of course H commutes with H itself, and therefore satisfies the law of conservation. But in the same way we see that A is a scalar quantity, i.e., is unchanged by rotation in space, if and only if it commutes with M, i.e., with the unitary operator induced in system space by the rotations in physical space. Now the energy H is certainly a scalar quantity, and consequently M commutes with H. But in accordance with what I have said above this means that M is constant in time; angular momentum satisfies the law of conservation.

I shall illustrate these very general and abstract considerations by the simplest case which fits into the general scheme: Schrödinger's scalar wave theory for a single particle. Let the rotation s carry the point $x\ y\ z$ over into $x'\ y'\ z'$; into what state ψ' does it carry the state ψ of our particle described by the Schrödinger function $\psi\ (x\ y\ z)$? Obviously this new state is defined by the equation

$$\psi'(x'y'z') = \psi(xyz). \tag{4}$$

If s is an infinitesimal rotation, the increments

$$\psi'(xyz)-\psi(xyz)=\delta\psi \text{ and } \delta x=x'-x$$

are all infinitesimals; our equation (4) then yields

$$\delta\psi+\left(\frac{\partial\psi}{\partial x}\,\delta x+\cdots\right)=0.$$

For the infinitesimal rotation (3) about the z-axis we get

$$\delta\psi=-\left(x\frac{\partial\psi}{\partial y}-y\frac{\partial\psi}{\partial x}\right)$$

and consequently M_z is the operator

$$L_z=\frac{1}{i}\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right) \tag{5}$$

and this is in complete agreement with the expression for angular momentum in classical dynamics:

$$L_z=xp_y-yp_x \tag{5*}$$

I believe that the validity of the conservation law and this agreement with classical mechanics affords sufficient justification for our definition of angular momentum.

A unitary vector space $\mathfrak{R}$ can be decomposed[1] into mutually perpendicular linear subspaces $\mathfrak{R}=\mathfrak{R}_1+\mathfrak{R}_2+\cdots$. That is to say, any vector $\mathfrak{x}$ in $\mathfrak{R}$ can be written in one and only one way as a sum $\mathfrak{x}_1+\mathfrak{x}_2+\cdots$ the individual summands of which lie in $\mathfrak{R}_1$, $\mathfrak{R}_2$, $\cdots$ respectively. For example, three-dimensional space can be decomposed into a plane and the line perpendicular to it. If we are given a linear unitary transformation of space, or a group of such transformations, we wish to carry out the decomposition in such a way that each of the subspaces $\mathfrak{R}_1$, $\mathfrak{R}_2$, $\cdots$ remains invariant under the given transformations; we further wish to carry it as far as possible under this condition. We then say: $\mathfrak{R}$ is decomposed into irreducible invariant sub-spaces with respect to the group under consideration. If, for example, we

[1] GQ, pp. 10-11.

have but a single infinitesimal unitary transformation the theorem on principal axes tells us that we can decompose into one-dimensional invariant sub-spaces—along the principal axes. The decomposition into irreducible invariant sub-spaces consequently corresponds to the separation of the various values which are possible for a physical quantity.

In particular, we consider the decomposition into invariant sub-spaces $\mathfrak{R}$ relative to the group of transformations which are induced in system space $\mathfrak{R}$ by the group of rotations in actual space. The rotation group then induces a definite representation Γ_j in each sub-space $\mathfrak{R}_j$. The operator representing moment of momentum is correspondingly separated into partial operators, each of which operates on one of the spaces $\mathfrak{R}_j$. At this point we use to advantage that discipline which the mathematicians call Topology or Analysis Situs. The rotations build a closed manifold, like the points on the surface of a sphere, and this has as consequence that there exists but a discrete set of different irreducible representations Γ_j of the group of rotations, which can be distinguished from one another by an index j which runs through the values $j=0, \frac{1}{2}, 1, \frac{3}{2}, \cdots$. The space $\mathfrak{R}_j$ in which the representation Γ_j with index j is induced has $2j+1$ dimensions. Consequently we know the moment of momentum M in $\mathfrak{R}_j$ independently of the dynamical structure of the physical system under consideration; its components are the operators which correspond to the infinitesimal rotations in the representation Γ_j. Computing the square of the absolute value M^2 we find that in $\mathfrak{R}_j$ this operator is simply multiplication by the constant $j(j+1)$. We thus come to the conclusion that the total system space $\mathfrak{R}$ can be decomposed into subspaces $\mathfrak{R}_j$ in such a way that

(1) $\mathfrak{R}_j$ has $2j+1$ dimensions;

(2) the energy in $\mathfrak{R}_j$ has a definite value E_j; and

(3) the square of the moment of momentum M^2 has the definite value $j(j+1)$.

j is called the inner quantum number of an atomic state represented by a vector lying in $\mathfrak{R}_j$. The infinitesimal displacement in time induces in system space the operator representing energy. Decomposition into invariant subspaces with respect to the group of actual displacements in time leads, therefore, to the principal axes of the energy operator. But since these displacements constitute an open group the various possible one-dimensional representations are not restricted *a priori* to a definite discrete set. This is the reason that we can give *a priori* definite discrete values of which the moment of momentum is capable, but not so in the case of the energy.

I must now mention as the last, the V-th quantum theoretic principle, that one which tells us how to effect the *composition of two physical systems*[1] into a single one. If (x_i) be an arbitrary vector in an m-dimensional space $\mathfrak{R}$, and (y_k) one such in an n-dimensional space $\mathfrak{R}'$, we can consider the $m \cdot n$ numbers $x_i y_k$ as the components of a vector $z = \mathfrak{x} \times \mathfrak{y}$ in an $(m \cdot n)$-dimensional space which I designate as the cross-product $\mathfrak{R} \times \mathfrak{R}'$. If the x_i be subjected to a linear transformation A and the y_k to B, then the $m \cdot n$ linearly independent quantities $x_i y_k$ undergo a certain linear transformation $A \times B$ induced in the product space $\mathfrak{R} \times \mathfrak{R}'$ by A in $\mathfrak{R}$ and B in $\mathfrak{R}'$. The rule of composition is: if $\mathfrak{R}$, $\mathfrak{R}'$ be the system spaces of the physical systems P, P' respectively, then $\mathfrak{R} \times \mathfrak{R}'$ is the system space of the total system composed of both P and P'. An operator A which represents a physical quantity of P in $\mathfrak{R}$ must be replaced by $A \times 1$ in order to represent the same quantity in the total system space $\mathfrak{R} \times \mathfrak{R}'$; $\times 1$ is here the identity in $\mathfrak{R}'$. This factor $\times 1$

[1] GQ, §17.

leaves all relations between the operators A undisturbed. Similarly, an operator B which represents a quantity of P' in $\mathfrak{R}'$, must be replaced by $1\times B$. It is thus possible to represent the quantities of P and P' by operators in the *same* system space $\mathfrak{R}\times\mathfrak{R}'$ without affecting the relations which exist between the quantities of either system. This is the situation intended when we say that the total physical system consists of two *kinematically independent parts*.

What influence has multiplicative composition on the infinitesimal operators? The equation

$$d(x_i y_k) = dx_i \cdot y_k + x_i \cdot dy_k$$

shows that the infinitesimal transformations

$$dx = Ax, \quad dy = By$$

in $\mathfrak{R}$ and $\mathfrak{R}'$ induce the infinitesimal transformation

$$(A\times 1)+(1\times B)$$

in the product space. In this sense infinitesimal operators behave additively on multiplicative composition.

Let the group γ of rotations induce representations

$$\mathfrak{U} : s\to U(s) \text{ in } \mathfrak{R}, \quad \mathfrak{U}' : s\to U'(s) \text{ in } \mathfrak{R}';$$

it therefore induces the representation

$$\mathfrak{U}'\times\mathfrak{U}' : s\to U(s)\times U'(s)$$

in product space $\mathfrak{R}\times\mathfrak{R}'$. Applying this to infinitesimal rotations and using the formula just derived for such we obtain the theorem: The moment of momentum of a physical system which consists of two kinematically independent parts is equal to the sum of the moments of momentum of the two partial systems. One might think that the same argument would hold for the operators in system space which give the infinitesimal displacement of the state vector in time, i.e., that the energy of the whole is equal to the sum of the energies of the parts. But there is an essential distinction between these two cases; the rotation in space is a virtual process, whereas the displacement in time describes what

actually happens. And this has as consequence that the law of the addition of energy only holds when the partial systems are dynamically, as well as kinematically, independent, i.e., when there is no interaction between them. The same theorem for angular momentum is not bound to this condition.

If the one part has an angular momentum whose magnitude is j and the other part j', then the angular momentum of the whole is, on classical mechanics, capable of all values between the limits $j+j'$ and $|j-j'|$. The various possibilities are conditioned by the various angles which the two moments, vectors of lengths j and j', can make with each other. What is the analogous problem in quantum mechanics? We must build the cross-product of the two irreducible representations Γ_j, $\Gamma_{j'}$ and decompose it into its irreducible constituents. The problem is solved by the formula[1]

$$\Gamma_j \times \Gamma_{j'} = \Sigma_\iota \Gamma_\iota$$

where ι takes on each of the values $j+j'$, $j+j'-1$, $\cdots$, $|j-j'|$ exactly once.

In order to follow the construction of an atom from electrons we will find it convenient to make use of a *vector model*, into which the angular momenta of the single electrons are introduced and added together in order to obtain the total. The mathematical interpretation given this model by quantum mechanics is characterized by the two circumstances:

(1) The determination of the various numerical possibilities is to be interpreted as decomposition into invariant irreducible sub-spaces;

(2) The addition of vectors has its mathematical counterpart in the multiplicative composition of the representations induced in these sub-spaces.

[1] GQ, §30.

This interpretation accounts for the following deviations from classical mechanics:

1) The inner quantum number j is restricted to the discrete values $0, \frac{1}{2}, 1, \frac{3}{2}, \cdots$;

2) The square of the absolute value of the angular momentum is $j(j+1)$ instead of j^2;

3) The inner quantum number obtained on composition is not capable of all values between $j+j'$ and $|j-j'|$, but only of those among them which differ from $j+j'$ by an integer.

In Schrödinger's wave theory the inner quantum number is only capable of integral values. This is, however, in disagreement with the observations on alkali spectra, which show a doublet with inner quantum numbers $j=l\pm\frac{1}{2}$ instead of a simple term with inner quantum number l. But if the wave function ψ has two components ψ_1, ψ_2 which depend on the coordinate system in such a way that under the influence of a rotation s they undergo that transformation which corresponds to s in the representation $\Gamma_{\frac{1}{2}}$, these facts are readily explained. The situation can be described by considering the single electron to consist in abstract of two kinematically independent parts, the electron translation and the electron spin.[1] The arguments (x, y, z) in ψ characterize the components in the system space associated with the translation and the indices 1, 2 the components in the two-dimensional system space associated with the spin. The angular momentum of translation is given by the classical formula (5); its inner quantum number is always integral and is called the azimuthal quantum number of the electron. The inner quantum number of the spin is $\frac{1}{2}$. If we distinguish in this way between the translatory angular momentum and the spin of each electron we arrive naturally

[1] GQ, §37.

at the Hund vector model of the atom which solved the problem of atomic line spectra with such a definite success. But this model is not to be taken literally; we obtain it in a new interpretation, in which the deviations 1)—3) from classical mechanics are explained from a unified viewpoint and not by hypotheses added *ad hoc*. This is the service rendered by the new quantum theory.

I have taken pains to show clearly the simple correspondence between the language of classical mechanics and that of quantum theory. There can be no doubt that to the same extent as the use of vectors, capable of all magnitudes and directions, and their additive composition were appropriate mathematical instruments for classical mechanics, so are decomposition into invariant sub-spaces relative to a given group and multiplicative composition of its representations the basic mathematical operations for the description of the same physical phenomena in the new mechanics. But far be it from me to exaggerate the importance of such a mathematical language. It is the same as with ordinary language; it is true that it can be of considerable assistance to thought, which should strictly be alone directed on the subject, in that it assists in fixing partial knowledge already won for further use. But it is also true that it entails the danger of carrying the spirit away from the subject proper into the void; poets and philosophers have occasionally made a virtue of such a predicament. But, after all, the clothing of physical relationships in a mathematical symbolism adapted for other purposes is not to be tolerated for long; hence it would be ungrateful of physics to refuse the valet service performed by mathematics in divesting it of an outworn and shabby garment. The foregoing is what I wish to present here for your consideration as an illustration of the applications of group theory to the new quantum mechanics.