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ROTATION OF A RIGID BODY IN QUANTUM MECHANICS

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ROTATION OF A RIGID BODY IN QUANTUM MECHANICS

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ACADEMISCH PROEFSCHRIFT

TER VERKRIJGING VAN DEN GRAAD VAN DOCTOR IN DE WIS- EN NATUURKUNDE AAN DE RIJKSUNIVERSITEIT TE LEIDEN, OP GEZAG VAN DEN RECTOR MAGNIFICUS Dr. J. J. BLANKSMA, HOOGLEERAAR IN DE FACULTEIT DER WIS- EN NATUURKUNDE, VOOR DE FACULTEIT DER WIS- EN NATUURKUNDE TE VERDEDIGEN OP DINSDAG 3 NOVEMBER 1931, DES NAMIDDAGS TE 4 UUR

DOOR

HENDRIK BRUGT GERHARD CASIMIR

GEBOREN TE 'S-GRAVENHAGE

promotor: Professor P. Ehrenfest

BIJ J. B. WOLTERS' UITGEVERS-MAATSCHAPPIJ N.V.
GRONINGEN, DEN HAAG, BATAVIA - 1931

RIJKS UNIVERSITEIT LEIDEN
INSTITUUT-LORENTZ

AAN MIJN OUDERS

Levensschets. 15 Julie 1909 werd ik te 's-Gravenhage geboren. Van 1915—1920 bezocht ik er de lagere school der Haagse schoolvereniging (direkteur de heer P. T. v. d. Meulen). In 1920 kwam ik op het Nederlands Lyceum, waar mijn vader toen nog rektor was. In 1925 deed ik er het eindeksamen H.B.S., het jaar daarop het eindeksamen gymnasium α. Het natuurkunde-onderwijs van de heer H. Corver maakte op mij een grote indruk. Graag zou ik ook Dr. G. Vrind danken voor zijn voortreffelike privaatlessen in de oude talen. Van de tegenwoordige rektor, de heer W. Reindersma, ondervond ik steeds warme belangstelling.

In 1926 ging ik naar Leiden. Ik volgde er de colleges in de wiskunde van prof. dr. J. C. Kluyver, prof. dr. W. v. d. Woude en prof. dr. J. Droste, die in de natuurkunde van mevr. dr. G. L. de Haas—Lorentz, prof. dr. W. J. de Haas en prof. dr. H. R. Woltjer, die in de astronomie van dr. J. Woltjer en het natuurkundig praktikum. Van 1927 af bezocht ik ook het natuurkundig colloquium van prof. dr. P. Ehrenfest; het spreekt wel van zelf, dat dit zeer veel voor mij heeft betekend. En dan wil ik nog de „ouderejaarsfles" noemen, die onder de uitnemende leiding van G. E. Uhlenbeck stond. Ik ben blij in deze tijd nog gelegenheid gehad te hebben een Maandagochtendcollege van prof. Lorentz bij te wonen. Junie 1928 deed ik het candidaatseksamen. Daarna was ik, samen met W. Blackstone, enige tijd in Göttingen. In September begon ik met de eigenlike studie der teoretiese natuurkunde. Ik volgde de colleges in wiskunde van prof. dr. J. C. Kluyver, prof. dr. W. v. d. Woude en prof. dr. J. A. Schouten, een college over relativiteitsteorie van prof. dr. A. D. Fokker. Maar het waren vooral de talrijke besprekingen met prof. Ehrenfest, die, steeds tot zelfstandig denken en verder werken aansporend, mij in de moderne teoretiese natuurkunde inleidden. In deze tijd werkte ik vooral samen met A. J. Rutgers. Voorjaar '29 ging ik samen met prof. Ehrenfest naar Kopenhagen, waar in het instituut voor teoretiese natuurkunde van prof. dr. N. Bohr een konferentie werd gehouden. Op uitnodiging van prof. Bohr bleef ik er tot de grote vakantie. Ook Sept.—Dec. '29, Febr.—April '30, Sept.—Dec. '30 was ik in Kopenhagen. Veel heb ik gehad aan de besprekingen en de vriendschappelike omgang met de vele fysici die hier voor kortere of

langere tijd werkten. Zo hebben opmerkingen van prof. dr. O. Klein veel bijgedragen tot de inhoud van dit proefschrift, dat ten dele een voortzetting van een van zijn publicaties is. Maar vooral het werken en de persoonlike omgang met prof. Bohr, maakten deze tijd voor mij zo belangrijk. Junie 1930 deed ik het doctoraaleksamen. Daarna vergezelden Rutgers en ik prof. Ehrenfest op zijn reis naar Amerika, waar hij aan de „university of Michigan" (Ann Arbor) een reeks colleges gaf. Ook prof. dr. E Fermi uit Rome gaf hier college. Voor deze reis mocht ik een ondersteuning ontvangen uit het Lorentzfonds. Begin 1931 had ik het voorrecht een maand assistent bij prof. Fokker te zijn. In Maart ging ik weer voor een maand naar Kopenhagen, waar het tienjarig jubileum van het instituut plechtig en feestelik werd herdacht. In Mei nam ik deel aan een congres te Zürich. In Sept. werd ik benoemd tot assistent bij prof. Ehrenfest.

Velen hebben tot mijn vorming bijgedragen, zowel op wetenschappelik gebied als anderszins. Maar aan prof. Ehrenfest en prof. Bohr heb ik in alle opzichten het meest te danken.

INTRODUCTION.

Classical mechanics knows two classes of systems: "material points" and "rigid bodies". In building up a general mathematical theory applying to any system, one usually starts from the equations of motion of a material point. From a physical point of view, however, the idea of "rigid body" is as fundamental a conception as the idea of "material point".

Quantum mechanics is primarily a description of the behaviour of elementary particles — electrons and nucleï — and of systems containing many of these particles, and its fundamental equations correspond to the classical equations of motion of a material point. Still it is possible to construct a quantum mechanics of the rigid body. The equations for the elementary particles are obtained from the corresponding classical equations by a definite mathematical procedure and this same procedure may be applied to the classical equations of the rigid body. The "mechanics of the rigid body" obtained this way, though lacking the fundamental physical importance of its classical analogon, is of interest as a mathematical formalism and also, as a paradigm of methods, useful in other problems in quantum mechanics. Fortunately it is of some direct physical importance, too. In dealing with molecules it is possible approximately to divide the motion into "internal motion" and rotation of the system as a whole, and, though it is necessary to investigate the problem more closely, we may expect that this rotation will be described by equations, only distinguished from the equations of the rigid body by such interaction terms, as do not influence the general mathematical treatment.

In this work an account of the quantum mechanics of the rigid body, or, as it is usually called, quantum mechanics of the "spinning top" is given.

In Chapter I we give a survey of the classical theory. As it must serve as a basis for the quantummechanical treatment, it contains some results, which are not found in ordinary textbooks on the subject, though, of course, it does not contain anything essentially new. In particular we have paid attention to the Poisson Brackets and their geometrical meaning, and to Lie's theorem on the connection between integrals and invariance of the Hamiltonian under infinitesimal canonical transformations.

Chapter II is devoted to the quantum mechanics of the rigid body. First we derive a wave equation from the equation for a system of many particles by *assuming* — in analogy to the corresponding classical deduction — that there is no interaction between internal motion and rotation. This wave equation was used by most authors on the subject. A more direct translation of classical theory is possible by means of matrix mechanics. The application of wave mechanics to our problem is due to Klein. It does not only have a formal advantage, it also offers a convenient way of calculating all quantities of physical importance. The algebraical solution of the matrix problem is worked out and a direct proof of the equivalence with wave mechanics is given. We do not investigate the wave functions more closely, since this has been done in many papers on the subject, especially in those of Kramers & Ittmann; some of the results on the assymmetrical top, however, are derived bij using simple properties of the wave functions. The chapter closes with a discussion of two-valued wave functions and their connection with spherical harmonics in fourdimensional space.

In Chapter III we show the connection of the results of [II] with the theory of the group of threedimensional rotations and its irreducible representations. Some of the methods used need a nearer justification, but especially the reasoning of [4], where an infinite representation is splitted up in its irreducible parts, is anything but rigorous.

Chapter IV is purely mathematical. In the first part we give an outline of the general theory of continuous groups. Theorems are stated only, not proved and even in the formulations no attempt to mathematical rigour is made. I have tried to describe,

what seemed to me the main lines of thought of the theory and to show that many of the results of the preceding chapters are special cases of general theorems. In the second part we derive a theorem, which is a generalisation of [III 3] and which seems to be of some mathematical interest,

In Chapter V we discuss the problem, how far it will be possible to describe the rotation of molecules by the equations of [II]. That it is possible approximately to separate the motion into internal motion and rotation was shown by Born and Oppenheimer, but we want to derive the *form* of the Hamiltonian, and to do this properly one ought to reproduce Born and Oppenheimer's argument, using explicit expressions for the various terms in the wave equation. I have, however, not been able to treat this general question and have confined myself to the discussion of the following problems:

B. The motion of a quantummechanical rigid body + a light particle (electron) with a potential energy depending on its position with respect to the rigid body.

A. The motion of a quantummechanical rigid body + a heavy particle (nucleus), bound by elastical forces to a certain point of the body.

The results obtained suggest a form of the rotational Hamiltonian for any molecule, involving six constants: the moments of inertia and a vector, representing the interaction between internal motion and rotation. One could try to apply this equation to the analysis of rotation bands. No such attempt has been made in this paper.

I.

CLASSICAL THEORY.

A. KINEMATICS.

1. Displacement-vectors.

A *change of position* of a rigid body is completely determined, if we know the displacement-vector for every point of the body. These displacement-vectors are of course not independent of each other for, the body being rigid, the distance between two arbitrary points must remain the same. It is possible to express them in terms of 6 parameters.

1, 1. Translations and rotations.

Every change of position can be composed of a *translation* (= change of position for which the displacement vector is the same for all points) and a *rotation* about an arbitrary point (= change of position which leaves this point at rest.) For let S be the initial, S' the final position of the point we will choose as centre of rotation. We may first carry out a translation which brings S to S'. To obtain the total change of position we have to add a rotation about S'. It is possible to choose for an arbitrary change of position the centre in such a way, that there is a simple connection between translations and rotations, but this is of no interest to us. Only if we take the centre of gravity of the body as centre of rotation, the kinematical decomposition into translations and rotations goes together with a decomposition of the dynamical equations, so that it is possible to treat rotation and translation as independent phenomena.

A translation is characterised by one displacement vector (three numbers!); to compose two translations we have simply to add these vectors.

1, 2. Rotations about an axis.
It may be seen from geometrical considerations, that whenever a change of position leaves at rest one point, that it leaves at rest all points of a straight line; a rotation about a point is always a rotation about an axis.

A rotation may accordingly be characterised by the axis of rotation — that is, a vector $\boldsymbol{a}$ with modul unity, $(\boldsymbol{a} \,.\, \boldsymbol{a}) = 1$ — and the angle ω through which the body is rotated; ω will be called positive, if an ordinary screw would move in the direction of $\boldsymbol{a}$ when submitted to the rotation. Together three parameters.

If one wants to have a one to one correspondence between rotations and parameters, one can take as parameters the numbers ωa_x, ωa_y, ωa_z and agree upon the following rules:

a. the absolute value of any of the three quantities must be less than 2π;

b. $0 \leqslant \omega a_z$; if $0 = \omega a_z$, $0 \leqslant \omega a_y$; if $0 = \omega a_z = \omega a_y$, $0 \leqslant \omega a_x$.

What is the displacement-vector for a point which before the rotation is given by the vector $\boldsymbol{r}$ drawn from the centre? The component in the direction of the axis, $(\boldsymbol{a} \,.\, \boldsymbol{r})\boldsymbol{a}$, remains the same; the component perpendicular to $\boldsymbol{a}$, $\boldsymbol{s} = \boldsymbol{r} - (\boldsymbol{a} \,.\, \boldsymbol{r})\boldsymbol{a}$, is rotated through an angle ω and (like every vector $\perp \boldsymbol{a}$) can be expressed after rotation as a linear combination of $\boldsymbol{s}$ and $[\boldsymbol{a} \times \boldsymbol{s}]$. One finds:

$$\boldsymbol{s}^* - \boldsymbol{s} = \sin\omega \,.\, [\boldsymbol{a} \times \boldsymbol{s}] - (1 - \cos\omega) \,.\, \boldsymbol{s}$$

which leads to:

(1) $$\boldsymbol{r}^* - \boldsymbol{r} = -(1 - \cos\omega)(\boldsymbol{r} - (\boldsymbol{a} \,.\, \boldsymbol{r})\boldsymbol{a}) + \sin\omega \,.\, [\boldsymbol{a} \times \boldsymbol{r}].$$

2. Multiplication of rotations.
Let R_1 and R_2 be two rotations. We define as the *product*, R_2R_1, the total rotation obtained by first carrying out R_1 and then R_2. From this definition follow at once the properties:

a. The product of two rotations is again a rotation.

b. The associative law of multiplication holds:
$R_3 \,.\, (R_2R_1) = (R_3R_2) \,.\, R_1$ (but in general: $R_2R_1 \neq R_1R_2$).

c. There exists an element E (unity) with the property $ER = RE = R$ for all R's. E is simply that "change of position" when nothing at all is changed.

d. To every rotation R corresponds a reciprocal one R^{-1}; $RR^{-1} = R^{-1}R = E$. A body that has been submitted to a rotation can always be brought back into the initial position. If R is the rotation $(\boldsymbol{a}, \omega)$, R^{-1} is the rotation $(\boldsymbol{a}, -\omega)$.

A set of elements for which multiplication is uniquely defined and for which the conditions $a - d$ are satisfied is called a *group*. The group of rotations is a *continuous group*, since the elements depend on three continuously varying parameters.

One will observe that also the rotations about one fixed axis form a group depending on one parameter. All elements of this *subgroup* commute with each other:

$$R(\boldsymbol{a}, \omega_1) \,.\, R(\boldsymbol{a}, \omega_2) = R(\boldsymbol{a}, \omega_1 + \omega_2) = R(\boldsymbol{a}, \omega_2) \,.\, R(\boldsymbol{a}, \omega_1)$$

such a group is called *Abelian*.

For general changes of position multiplication may be defined in exactly the same way as was done for rotations and also they form a group.

2, 1. Description in rectangular coordinates.
Instead of using the vector notation of [1, 2] we may introduce a system of rectangular coordinates with its origin in the centre of rotation. If we call x_i the coordinates of a point before a rotation $(\boldsymbol{a}, \omega)$, x_i^* the coordinates after this rotation it follows from [1, 2 (1)] that we will have relations of the form:

(1*a*) $$x_i^* = \sum_l \mathrm{A}_{il}(\boldsymbol{a}, \omega) \,.\, x_l$$

(compare also [3]). Symbolically we may write:

(1*b*) $$\boldsymbol{x}^* = \mathrm{A}\boldsymbol{x};$$

the symbol $\boldsymbol{x}$ may be interpreted as a matrix with only one column.

If we carry out a second rotation $(\boldsymbol{a}', \omega')$ we will have:

(2a) $x_i^{**} = \sum_m A_{im}(\boldsymbol{a}', \omega') . x_m^{*} = \sum_m \sum_n A_{im}(\boldsymbol{a}', \omega') . A_{mn}(\boldsymbol{a}, \omega) . x_n$

symbolically:

(2b) $$\boldsymbol{x}^{**} = A(\boldsymbol{a}', \omega') . A(\boldsymbol{a}, \omega) . \boldsymbol{x}$$

to the product of two rotations corresponds the product of the matrices in the same order. (Perhaps we should rather say: the multiplication of a matrices is defined so that this condition is satisfied.)

2, 2. Translations and rotations.

Geometrically it is evident: when we first carry out a translation, which brings the centre of the body from C to C' and then a rotation $(\boldsymbol{a}, \omega)$ about C', the result is the same as if we first carry out a rotation $(\boldsymbol{a}, \omega)$ about C and then the translation $C \rightarrow C'$. Thus we may interchange rotations and translations.

Consider a succession of changes of position, $R_2 . T_2 . R_1 . T_1$ (R rotation, T translation). T_1 brings $C \rightarrow C'$, T_2 brings $C' \rightarrow C''$; R_1 is the rotation $(\boldsymbol{a}_1, \omega_1)$ about C', R_2 the rotation $(\boldsymbol{a}_2, \omega_2)$ about C''; the final result is just the same as if we first carry out the translation $C \rightarrow C''$ and then the rotation $R(\boldsymbol{a}_2, \omega_2) . R(\boldsymbol{a}_1, \omega_1)$ about C''.

If we always choose as centre of rotation the same point of the body (not the same point in space!) we can multiply the rotations that form part of the general changes of position as if there were no translations at all.

If we use the matrix formulation we have:

If we describe every rotation in a system of coordinates having its origin always in the same point of the body and having axes parallel to a certain "standard-system", these matrices must be multiplied in the same order in which the rotations are carried out, in order to get the matrix describing the rotation which, together with the sum of all translations, forms the resultant change of position.

3. Nearer investigation of the description in rectangular coordinates.

We will use a system of coordinates for which a motion from

the positive x-axis towards the positive y-axis corresponds to a positive rotation about the z-axis. For the components of the vectorial product, $\boldsymbol{c} = [\boldsymbol{a} \times \boldsymbol{b}]$, defined with help of the screw-rule we then have: $c_x = a_y b_z - a_z b_y$ etc. We call the vectors of unit length in the direction of the axes $\boldsymbol{f}_1$, $\boldsymbol{f}_2$, $\boldsymbol{f}_3$; we have:

(1) $$\boldsymbol{f}_1 = [\boldsymbol{f}_2 \times \boldsymbol{f}_3]; \quad \boldsymbol{f}_2 = [\boldsymbol{f}_3 \times \boldsymbol{f}_1]; \quad \boldsymbol{f}_3 = [\boldsymbol{f}_1 \times \boldsymbol{f}_2].$$

(2) $$(\boldsymbol{f}_1 . \boldsymbol{f}_1) = (\boldsymbol{f}_2 . \boldsymbol{f}_2) = (\boldsymbol{f}_3 . \boldsymbol{f}_3) = 1.$$

Formula [1,2 (1)] gives:

(3)
$$\begin{aligned} x^* &= (\cos\omega + (1-\cos\omega) . a_x^2)x + ((1-\cos\omega) . a_x a_y - \sin\omega . a_z)y + \\ &\quad + ((1-\cos\omega) . a_x a_z + \sin\omega . a_y)z \\ y^* &= ((1-\cos\omega) . a_y a_x + \sin\omega . a_z)x + (\cos\omega + (1-\cos\omega) . a_y^2)y + \\ &\quad + ((1-\cos\omega) . a_y a_z - \sin\omega . a_x)z \\ z^* &= ((1-\cos\omega) . a_z a_x - \sin\omega . a_y)x + \\ &\quad ((1-\cos\omega) . a_z a_y + \sin\omega . a_x)y + (\cos\omega + (1-\cos\omega) a_z^2)z. \end{aligned}$$

This may be brought into a much more symmetrical form by introducing the parameters:

(4) $$\xi = \sin\frac{\omega}{2} . a_x; \quad \eta = \sin\frac{\omega}{2} . a_y; \quad \zeta = \sin\frac{\omega}{2} . a_z; \quad \chi = \cos\frac{\omega}{2}.$$

They satisfy the relations:

(5) $$\xi^2 + \eta^2 + \zeta^2 + \chi^2 = 1.$$

Our equations become:

(6)
$$\begin{aligned} x^* &= (\chi^2 + \xi^2 - \eta^2 - \zeta^2)x + 2(\xi\eta - \chi\zeta)y + 2(\xi\zeta + \chi\eta)z \\ y^* &= 2(\xi\eta + \chi\zeta)x + (\chi^2 + \eta^2 - \xi^2 - \zeta^2)y + 2(\eta\zeta - \chi\xi)z \\ z^* &= 2(\xi\zeta - \chi\eta)x + 2(\eta\zeta + \chi\xi)y + (\chi^2 + \zeta^2 - \xi^2 - \eta^2)z. \end{aligned}$$

To these parameters we will return later on.

3, 1. Transformation coefficients as cosines.

As already remarked in [2, 1] the transformation [3 (3)] is of the form:

(1) $$x_n^* = \sum_m k_{nm} x_m.$$

To make clear the geometrical meaning of the k_{mn}, we introduce a system of axes fixed in the body, which before the rotation

falls together with the $\boldsymbol{f}_i$. The point which before the rotation has the coordinates $x_1 = 1$, $x_2 = x_3 = 0$ will after the rotation have the coordinates k_{11}, k_{21}, k_{31}. It follows: k_{i1} is the cosine of the angle between $\boldsymbol{f}_i$ and the x-axis of the system fixed in the body. Analogously for k_{i2} and k_{i3}. If we call $\boldsymbol{k}'_i$ the vector of unit length in the direction of the axes fixed in the body after rotation, we have:

(2) $$k_{nm} = (\boldsymbol{f}_n \,.\, \boldsymbol{k}'_m).$$

As the $\boldsymbol{k}'_i$'sare perpendicular to each other, we have:

(3*b*) $$(\boldsymbol{k}'_m \,.\, \boldsymbol{k}'_l) = \delta_{ml}$$

or

(3*a*) $$\sum_i k_{im} k_{il} = \delta_{ml}.$$

Further:

(4) $$\boldsymbol{k}'_3 = [\boldsymbol{k}'_1 \times \boldsymbol{k}'_2] \qquad \text{etc.}$$

(5) $$(\boldsymbol{k}'_3 \,.\, [\boldsymbol{k}'_1 \times \boldsymbol{k}'_2]) = \text{Det}\,(k_{nm}) = +1.$$

On the other hand every transformation satisfying (3*a*) and (5) is a rotation. For these equations mean, that we have three vectors, perpendicular to each other and numbered in such a way that $\boldsymbol{k}'_3 = [\boldsymbol{k}'_1 \times \boldsymbol{k}'_2]$; these vectors can therefore be regarded as fundamental vectors of a system of coordinate axes.

It follows from (3*a*) and also from [3 (3)]:
The matrix describing the rotation reciprocal to that described by $\| k_{nm} \|$ is obtained by interchanging rows and columns.

(6) $$(k^{-1})_{mn} = k_{nm}.$$

3, 2. Transformation of coordinates.

Our $\boldsymbol{f}$-system may of course be chosen arbitrarily and the formula $\boldsymbol{x}^* = \mathrm{K}\boldsymbol{x}$ does not only describe a rotation of the body but may also be interpreted as a rotation of the $\boldsymbol{f}$-system, while the $\boldsymbol{k}'$-system keeps the same orientation in space. The matrix K only tells about the relative position of two systems of axes.

Only if we also consider points not moving along with the body there is a difference. There is also a difference if we treat the problem of the motion in an external field, when a rotation

does not change the components of the external field and a transformation of coordinates does.

Let A be a matrix describing a rotation in a certain $\boldsymbol{f}$-system, $\boldsymbol{x}^* = \mathrm{A}\boldsymbol{x}$. If $\boldsymbol{y} = \mathrm{T}\boldsymbol{x}$ is a transformation of coordinates we find for the rotation in the new coordinate-system:

(1) $$\boldsymbol{y}^* = \mathrm{T}\boldsymbol{x}^* = \mathrm{TA}\boldsymbol{x} = \mathrm{TAT}^{-1}\boldsymbol{y}.$$

From this it follows that two rotations. A and TAT^{-1} belong to the same value of ω (but to different $\boldsymbol{a}$!). For one can always find a system of coordinates such that the second rotation looks just the same as the first one in the original system. But a transformation of coordinates changes only the a_i, not ω. In group theory the elements BAB^{-1} (A fixed, B all elements) are said to form a *class*. The rotations through a fixed angle, about arbitrary axes form a class.

3, 3. Moving system of axes.

In describing a rotation we used an $\boldsymbol{f}$-system fixed in space. And to describe a succession of rotations we have to introduce a new $\boldsymbol{k}'$-system for every rotation. On the other hand, in separating translations from rotations we always chose the same point of the body as centre of rotation. We may do something analogous for the rotations: besides the $\boldsymbol{f}$-system we introduce a $\boldsymbol{k}$-system, fixed in the body and keeping the same orientation with respect to the body, for whatever changes of position we carry out.

It is clear that we have to do something of this kind if we do not only want to speak about changes of position, but also about position itself. Once there has been chosen a $\boldsymbol{k}$-system there is a certain "normal" position in which the $\boldsymbol{k}$- and $\boldsymbol{f}$-system fall together, and an arbitrary position is determined by the rotation which brings the body from the normal into the new position, the transformation matrix being given by $k_{nm} = (\boldsymbol{f}_n \,.\, \boldsymbol{k}_m)$.

If we have not only rotations but general changes of position, one will again fix a "normal" position. To bring the body into another position one will first carry out a translation which brings the centre into the right point in space, and then a

rotation. The "*orientation*" will now be determined by the projections of the $\boldsymbol{k}$-axes on axes through the centre parallel to the normal ones.

It is now possible to describe a rotation in an $\boldsymbol{f}'$-system which before the rotation falls together with the $\boldsymbol{k}$-system. The transformation matrix is then given by $(\boldsymbol{f}'_n \,.\, \boldsymbol{k}_m)$, ($\boldsymbol{k}_m$ being the $\boldsymbol{k}$-vectors after rotation). It may also be obtained by applying [3 (3)]; for the a_i, one must then take the components in the $\boldsymbol{f}'$-system, that is, the expressions $(\boldsymbol{k}_i \,.\, \boldsymbol{a})$ before the rotation. Somewhat unexactly we will speak about a "description in the moving system".

Let us consider two rotations, R_1, R_2, the first one described by M_1, the second one by M_2 in the moving system. We want to determine the matrix describing R_2R_1 in the moving system. The $\boldsymbol{f}'$-system is the same for R_2R_1 as for R_1, but in this system R_2 is not described by M_2 but by $M_1M_2M_1^{-1}$. Thus R_2R_1 is described by $M_1M_2M_1^{-1} \,.\, M_1 = M_1M_2$: the order of the factors is reversed. This result may also be obtained from the formulae.

$$(M_2)_{mn} = (\boldsymbol{f}''_m \,.\, \boldsymbol{k}_n); \quad (M_1)_{pm} = (\boldsymbol{f}'_p \,.\, \boldsymbol{f}''_m); \quad (M_{R_2R_1})_{pn} = (\boldsymbol{f}'_p \,.\, \boldsymbol{k}_n).$$

(We have spoken already about the possibility of changing the $\boldsymbol{f}$-system. We can however also change the $\boldsymbol{k}$-system. The matrix determining the position, $k_{nm} = (\boldsymbol{f}_n \,.\, \boldsymbol{k}_m)$ will be changed in exactly the same way whether we really rotate the body or whether only the $\boldsymbol{k}$-system is rotated the body remaining at rest. Also for points and vectors not connected with the body (external field) the transformations are the same. They are however different for the points of the body itself: in the case of rotation of the body the coordinates of these points in the $\boldsymbol{f}$-system will change, the coordinates in the $\boldsymbol{k}$-system remaining the same; in the case of a change of the $\boldsymbol{k}$-system it is just the reverse. One will see that there is a complete symmetry between the two systems. And it is more for symmetry's sake then because of the real importance of the result that all these possibilities are mentioned.)

Of course a "rotation defined in the moving system" may also be interpreted as a change of $\boldsymbol{f}$-system. In which way a rotation (or change of $\boldsymbol{f}$-system) that in the $\boldsymbol{k}$-system is given

by M_k will be described in the $\boldsymbol{f}$-system depends on the position. If the position is given by $\|K_{nm}\|$ we will have:

$$M_f = KM_kK^{-1}.$$

If we next carry out a rotation, described by L_f in the $\boldsymbol{f}$-system, the final result is: $L_f \,.\, KM_kK^{-1}$. If we first carry out L_f we have: $M_f = L_fKM_kK^{-1}L_f^{-1}$, and the final result is again: $L_f \,.\, KM_kK^{-1}$. In this sense rotations defined in the $\boldsymbol{k}$-system commute with rotations defined in the $\boldsymbol{f}$-system.

4. The Eulerian angles.

In [3] we expressed the nine K_{nm} in terms of a_i and ω. This way of describing a rotation has the advantage that it is possible at once to write down the transformation-matrix in an arbitrary system of coordinates. One must only know the components of $\boldsymbol{a}$ in this system. But for actual applications, where the problem is: determine the position as function of the time, an other set of parameters is much more convenient.

Let the coordinates in the $\boldsymbol{f}$-system be called x^*, y^*, z^* in the $\boldsymbol{k}$-system x, y, z and let s be the line of intersection of the x^*, y^* and the x, y plane (s is the common perpendicular on $\boldsymbol{k}_z$ and $\boldsymbol{f}_z$). We call:

ϑ the angle between z^*-and z-axis.
ψ the angle between x^*-axis and s
φ the angle between s and x-axis

(Frequently we will write instead of ϑ, ψ, φ, ϑ^1, ϑ^2, ϑ^3). We will always assume $0 \leqslant \vartheta \leqslant \pi$. The positive direction on s will be chosen so as to make the transition $z^* \to z$ correspond to a positive rotation about s. ψ is positive if the transition $x^* \to s$ corresponds to a positive rotation about the z^*-axis. In the same way φ is positive if $s \to x$ is a positive rotation about the z-axis.

Our definitions may also be expressed by the formulae

(1a, b, c) $\quad 0 \leqslant \vartheta \leqslant \pi; \quad 0 \leqslant \psi < 2\pi; \quad 0 \leqslant \varphi < 2\pi.$

(2) $\qquad \cos\vartheta = (\boldsymbol{k}_z \,.\, \boldsymbol{f}_z).$

(3) $$\sin\vartheta \,.\, \boldsymbol{s} = [\boldsymbol{f}_z \times \boldsymbol{k}_z].$$

(4) $$\sin\psi \,.\, \boldsymbol{f}_z = [\boldsymbol{f}_x \times \boldsymbol{s}].$$

(5) $$\sin\varphi \,.\, \boldsymbol{k}_z = [\boldsymbol{s} \times \boldsymbol{k}_x].$$

We can now directly determine the projections $(\boldsymbol{f}_n \,.\, \boldsymbol{k}_m)$. But there is still another way of finding the K-matrix. The rotation that brings the body from the normal position into the final one, may be built up in the following way:

1°. rotation about $\boldsymbol{f}_z$ through ψ,

2°. rotation about $\boldsymbol{s}$ through ϑ,

3°. rotation about $\boldsymbol{k}_z$ through φ,

or also (as is seen by describing the three rotations in the $\boldsymbol{k}$-system and observing that we then must reverse the order of multiplication):

1°. rotation about $\boldsymbol{f}_z$ through φ,

2°. rotation about $\boldsymbol{f}_x$ through ϑ,

3°. rotation about $\boldsymbol{f}_z$ through ψ.

We must multiply the matrices belonging to these three rotations:

(6) $$\|K_{nm}\| = \begin{Vmatrix} \cos\psi & -\sin\psi & 0 \\ \sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{Vmatrix} . \begin{Vmatrix} 1 & 0 & 0 \\ 0 & \cos\vartheta & -\sin\vartheta \\ 0 & \sin\vartheta & \cos\vartheta \end{Vmatrix} . \begin{Vmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{Vmatrix}$$

One finds:

(7)

	$\boldsymbol{k}_x$	$\boldsymbol{k}_y$	$\boldsymbol{k}_z$
$\boldsymbol{f}_x$	$\cos\psi.\cos\varphi - \cos\vartheta.\sin\varphi.\sin\psi$	$-\cos\psi.\sin\varphi - \cos\vartheta.\cos\varphi.\sin\psi$	$\sin\psi.\sin\vartheta$
$\boldsymbol{f}_y$	$\sin\psi.\cos\varphi + \cos\vartheta.\sin\varphi.\cos\psi$	$-\sin\psi.\sin\varphi + \cos\vartheta.\cos\varphi.\cos\psi$	$-\cos\psi.\sin\vartheta$
$\boldsymbol{f}_z$	$\sin\vartheta.\sin\varphi$	$\sin\vartheta.\cos\varphi$	$\cos\vartheta$

When the position is first determined by: $(\boldsymbol{f}_n \,.\, \boldsymbol{k}_m) = K_{nm}(\vartheta^\nu)$ and a rotation defined by ζ^ν in the $\boldsymbol{f}$-system is carried out, we will have after the rotation:

$$K(\zeta^\nu) \,.\, K(\vartheta^\lambda) = K(\vartheta^{*\lambda})$$

where $\vartheta^{*\lambda}$ is a function of ϑ^{λ}, ζ^{ν}:

$$\vartheta^{*\lambda} = g^{\lambda}(\zeta^{\nu}, \vartheta^{\mu}).$$

The functions g^{λ} are rather complicated; we do not want to determine them.

Important is the connection between polar coordinates and the Eulerian angles: ϑ and $\psi - \frac{\pi}{2}$ are the polar coordinates of $\boldsymbol{k}_z$ in the $\boldsymbol{f}$-system; ϑ and $\varphi + \frac{\pi}{2}$ the polar coordinates of $\boldsymbol{f}_z$ in the $\boldsymbol{k}$-system.

5. Quaternions.

We introduce three units, j, k, l (sometimes we write k_1, k_2, k_3) for which the following relations are assumed to hold:

(1a) $$j^2 = k^2 = l^2 = -1;$$

(1b) $$j.k = -k.j = l, \quad k.l = -l.k = j; \quad l.j = -j.l = k.$$

Together with the number 1 they form the basis of an algebra: for the "numbers" of the form $a_0 + a_1 . j + a_2 . k + a_3 . l$ (a_i an ordinary number) we can define addition and multiplication, so that the result is again a number of the same form and all laws hold except the commutative law of multiplication.
Addition:

$$(a_0 + \sum_i a_i . k_i) + (b_0 + \sum_i b_i . k_i) = (a_0 + b_0 + \sum_i (a_i + b_i) k_i).$$

Multiplication with an ordinary number:

$$\alpha(a_0 + \sum_i a_i . k_i) = \alpha a_0 + \sum_i (\alpha a_i) . k_i.$$

Multiplication:

$$(a_0 + a_1 . j + a_2 . k + a_3 . l)(b_0 + b_1 . j + b_2 . k + b_3 . l) =$$
$$= a_0 . b_0 + a_0 b_1 . j + \ldots + a_1 b_0 . j + a_1 b_1 . j^2 + \ldots + \ldots$$

(one works out the brackets using the distributive law of multiplication but not changing the order of the factors k_i).

The "numbers" $a_0 + \sum_i a_i \,.\, k_i$ are called *quaternions*. If a_i is real also division is possible, for

$$(2) \qquad (a_0 + \sum a_i \,.\, k_i) \,.\, \frac{1}{\sum (a_i)^2 + {a_0}^2} (a_0 - \sum a_i \,.\, k_i) = 1.$$

5, 1. Quaternions and vectors. Rotations.
We will associate with a vector (a_1, a_2, a_3) the quaternion $a_1 \,.\, j + a_2 \,.\, k + a_3 \,.\, l$; we write:

$$(1) \qquad \mathfrak{a} = a_1 \,.\, j + a_2 \,.\, k + a_3 \,.\, l.$$

Using this notation we find for the product of two quaternions:

$$(2) \qquad (a_0 + \mathfrak{a})(b_0 + \mathfrak{b}) = a_0 b_0 - (\boldsymbol{a} \,.\, \boldsymbol{b}) + a_0 \,.\, \mathfrak{b} + b_0 \,.\, \mathfrak{a} + [\mathfrak{a} \times \mathfrak{b}].$$

The importance of quaternions for the kinematics of rotations is due to the following theorem:

Let $\boldsymbol{r}^*$ be the radius vector of a point, the position of which was initially given by $\boldsymbol{r}$, after a rotation $(\boldsymbol{a}, \omega)$. Then:

$$(2) \qquad \mathfrak{r}^* = (\cos \frac{\omega}{2} + \sin \frac{\omega}{2} \,.\, \mathfrak{a}) \,.\, \mathfrak{r} \,.\, (\cos \frac{\omega}{2} - \sin \frac{\omega}{2} \,.\, \mathfrak{a}).$$

The quaternions on the left and the right are reciprocal to each other. The first one is: $\chi + \xi \,.\, j + \eta \,.\, k + \zeta \,.\, l$ where ξ, η, ζ, χ are the quantities defined in [3]. (3) is easily proved by twice applying (2); we arrive automatically at [3 (3)]. (Of course one can also show that the transformation is given by [3 (6)]).

Consider two rotations $(\boldsymbol{a}_1, \omega_1)$, $(\boldsymbol{a}_2, \omega_2)$. To the product $R_2 R_1$ belongs the quaternion:

$$(4) \qquad \begin{aligned} &\cos \frac{\omega_1}{2} \,.\, \cos \frac{\omega_2}{2} - \sin \frac{\omega_1}{2} \,.\, \sin \frac{\omega_2}{2} \,.\, (\boldsymbol{a}_1 \,.\, \boldsymbol{a}_2) + \\ &+ \cos \frac{\omega_1}{2} \,.\, \mathfrak{a}_2 + \cos \frac{\omega_2}{2} \,.\, \mathfrak{a}_1 + \sin \frac{\omega_1}{2} \,.\, \sin \frac{\omega_2}{2} \,.\, [\mathfrak{a}_2 \times \mathfrak{a}_1]. \end{aligned}$$

This formula determines axis and angle for the resultant rotation. For ξ, η, ζ, χ one finds:

$$(5) \qquad \begin{aligned} \xi &= \chi_1 \xi_2 + \chi_2 \xi_1 + \eta_2 \zeta_1 - \zeta_2 \eta_1 \\ \eta &= \chi_1 \eta_2 + \chi_2 \eta_1 + \zeta_2 \xi_1 - \xi_2 \zeta_1 \\ \zeta &= \chi_1 \zeta_2 + \chi_2 \zeta_1 + \xi_2 \eta_1 - \eta_2 \xi_1 \\ \chi &= \chi_1 \chi_2 - \xi_1 \xi_2 - \eta_1 \eta_2 - \zeta_1 \zeta_2. \end{aligned}$$

5, 2. Two-valuedness of the ξ, η, ζ, χ.
The ξ, η, ζ, χ are no one-valued parameters: ξ, η, ζ, χ and $-\xi, -\eta, -\zeta, -\chi$ correspond to the same rotation. But an advantage is that they depend continuously on the rotations (positions): if we describe a certain position by ξ_i, a second position near it *can* be described by parameters ξ_i', such that the differences $|\xi_i - \xi_i'|$ are small. The Eulerian angles do not have this property for positions near the normal one.

We can make the ξ_i's, one-valued by the rules of [1, 2] but then we disturbe the continuity.

5, 3. Connection between ϑ^ν and ξ_i:
To a rotation defined by ϑ, φ, ψ belongs a quaternion (see [4]):

$$(1) \qquad (\chi + \sum \xi_i k_i) = (\cos \frac{\psi}{2} + \sin \frac{\psi}{2} \,.\, l)(\cos \frac{\vartheta}{2} + \sin \frac{\vartheta}{2} \,.\, j)(\cos \frac{\varphi}{2} + \sin \frac{\varphi}{2} \,.\, l).$$

It follows:

$$(2) \qquad \begin{aligned} \xi &= \cos \frac{\psi}{2} \,.\, \cos \frac{\varphi}{2} \,.\, \sin \frac{\vartheta}{2} + \sin \frac{\psi}{2} \,.\, \sin \frac{\varphi}{2} \,.\, \sin \frac{\vartheta}{2} = \cos \frac{\psi - \varphi}{2} \,.\, \sin \frac{\vartheta}{2} \\ \eta &= \sin \frac{\psi}{2} \,.\, \cos \frac{\varphi}{2} \,.\, \sin \frac{\vartheta}{2} - \cos \frac{\psi}{2} \,.\, \sin \frac{\varphi}{2} \,.\, \sin \frac{\vartheta}{2} = \sin \frac{\psi - \varphi}{2} \,.\, \sin \frac{\vartheta}{2} \\ \zeta &= \cos \frac{\psi}{2} \,.\, \sin \frac{\varphi}{2} \,.\, \cos \frac{\vartheta}{2} + \sin \frac{\psi}{2} \,.\, \cos \frac{\varphi}{2} \,.\, \cos \frac{\vartheta}{2} = \sin \frac{\psi + \varphi}{2} \,.\, \cos \frac{\vartheta}{2} \\ \chi &= \cos \frac{\psi}{2} \,.\, \cos \frac{\varphi}{2} \,.\, \cos \frac{\vartheta}{2} - \sin \frac{\psi}{2} \,.\, \sin \frac{\varphi}{2} \,.\, \cos \frac{\vartheta}{2} = \cos \frac{\psi + \varphi}{2} \,.\, \cos \frac{\vartheta}{2}. \end{aligned}$$

6. Infinitesimal rotations.
If the angle of rotation becomes smaller and smaller we need in the limit only take into account the first power. [1,2 (1)] then becomes:

$$(1) \qquad \boldsymbol{r}^* - \boldsymbol{r} = \delta\omega \,.\, [\boldsymbol{a} \times \boldsymbol{r}].$$

If we carry out a second infinitesimal rotation we find:

(2) $\boldsymbol{r}^* - \boldsymbol{r} = \delta\omega_1 . [\boldsymbol{a}_1 \times \boldsymbol{r}] + \delta\omega_2 . [\boldsymbol{a}_2 \times \boldsymbol{r}] = [(\delta\omega_1 . \boldsymbol{a}_1 + \delta\omega_2 . \boldsymbol{a}_2) \times \boldsymbol{r}]$;

infinitesimal rotations have the character of vectors: to find the result of two such rotations one has simply to add the corresponding vectors. Every infinitesimal rotation can be decomposed into rotations about the coordinate axes; of course one can again decompose in the $\boldsymbol{f}$- or the $\boldsymbol{k}$- (better $\boldsymbol{f}'$-)system. We write:

(3) $$\boldsymbol{x}^* - \boldsymbol{x} = \varepsilon \mathrm{D}_i \boldsymbol{x}$$

when an infinitesimal rotation ε about the i-axis is carried out. The D_i are then given by:

(4a,b,c) $$\mathrm{D}_1 = \begin{Vmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{Vmatrix};\ \mathrm{D}_2 = \begin{Vmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{Vmatrix};\ \mathrm{D}_3 = \begin{Vmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{Vmatrix}.$$

To an infinitesimal rotation $\delta\omega . \boldsymbol{a}$ belongs the matrix:

(5) $$\mathrm{M} = 1 + \delta\omega . \sum_i a_i \mathrm{D}_i.$$

6, 1. Properties of the $\boldsymbol{D_i}$.
In another coordinate system [6 (5)] becomes:

(1a) $$\mathrm{M}^* = 1 + \sum_{i,k} \mathrm{A}_{ik} a_k \mathrm{D}_i;$$

On the other hand:

(1b) $$\mathrm{M}^* = \mathrm{AMA}^{-1},$$

consequently:

$$\mathrm{AD}_k\mathrm{A}^{-1} = \sum_i \mathrm{A}_{ik}\mathrm{D}_i = \sum_i (\mathrm{A}^{-1})_{ki}\mathrm{D}_i$$

or, writing A for A^{-1}:

(2) $$\mathrm{A}^{-1}\mathrm{D}_k\mathrm{A} = \sum_i \mathrm{A}_{ki}\mathrm{D}_i.$$

It is easy to verify this relation when also A is an infinitesimal rotation. We have to use the relations:

(3)
$$\begin{aligned} \mathrm{D}_1\mathrm{D}_2 - \mathrm{D}_2\mathrm{D}_1 &= \mathrm{D}_3 \\ \mathrm{D}_2\mathrm{D}_3 - \mathrm{D}_3\mathrm{D}_2 &= \mathrm{D}_1 \\ \mathrm{D}_3\mathrm{D}_1 - \mathrm{D}_1\mathrm{D}_3 &= \mathrm{D}_2. \end{aligned}$$

6, 2. Infinitesimal rotations and Eulerian angles.
In which way do the Eulerian angles, that determine the position, change when an infinitesimal rotation about $\boldsymbol{f}_i$ resp. $\boldsymbol{k}_i$ is carried out? And what are the components of a rotation which brings the body from the position ϑ^ν into the position $\vartheta^\nu + d\vartheta^\nu$?

We will first answer the second question. To the rotations defined by $d\vartheta$, $d\varphi$, $d\psi$ belong certain vectors: $d\vartheta\boldsymbol{g}_\vartheta$, $d\varphi\boldsymbol{g}_\varphi$, $d\psi\boldsymbol{g}_\psi$. We have (see [4]):

$$\begin{aligned} \boldsymbol{g}_\vartheta &= \boldsymbol{s} = \frac{1}{\sin\vartheta}[\boldsymbol{f}_z \times \boldsymbol{k}_z] \\ \boldsymbol{g}_\varphi &= \boldsymbol{k}_z \\ \boldsymbol{g}_\psi &= \boldsymbol{f}_z. \end{aligned}$$

Thus we have:

(1A, B)
$$\begin{aligned} \boldsymbol{g}_\vartheta &= \cos\psi . \boldsymbol{f}_x + \sin\psi . \boldsymbol{f}_y = \cos\varphi . \boldsymbol{k}_x - \sin\varphi . \boldsymbol{k}_y \\ \boldsymbol{g}_\psi &= \boldsymbol{f}_z = \sin\vartheta . \sin\varphi . \boldsymbol{k}_x + \sin\vartheta . \cos\varphi . \boldsymbol{k}_y + \cos\vartheta . \boldsymbol{k}_z \\ \boldsymbol{g}_\varphi &= \sin\vartheta . \sin\psi . \boldsymbol{f}_x - \sin\vartheta . \cos\psi . \boldsymbol{f}_y + \cos\vartheta . \boldsymbol{f}_z = \boldsymbol{k}_z. \end{aligned}$$

By solving these equations for $\boldsymbol{f}_i$ resp. $\boldsymbol{k}_i$ we get:

(2)
$$\begin{aligned} \boldsymbol{f}_x &= \cos\psi . \boldsymbol{g}_\vartheta - \frac{\cos\vartheta . \sin\psi}{\sin\vartheta} \cdot \boldsymbol{g}_\psi + \frac{\sin\psi}{\sin\vartheta} \cdot \boldsymbol{g}_\varphi \\ \boldsymbol{f}_y &= \sin\psi . \boldsymbol{g}_\vartheta + \frac{\cos\vartheta . \cos\psi}{\sin\vartheta} \cdot \boldsymbol{g}_\psi - \frac{\cos\psi}{\sin\vartheta} \cdot \boldsymbol{g}_\varphi \\ \boldsymbol{f}_z &= \boldsymbol{g}_\psi \end{aligned}$$

(3)
$$\begin{aligned} \boldsymbol{k}_x &= \cos\varphi . \boldsymbol{g}_\vartheta + \frac{\sin\varphi}{\sin\vartheta} \cdot \boldsymbol{g}_\psi - \frac{\cos\vartheta . \sin\varphi}{\sin\vartheta} \cdot \boldsymbol{g}_\varphi \\ \boldsymbol{k}_y &= -\sin\varphi . \boldsymbol{g}_\vartheta + \frac{\cos\varphi}{\sin\vartheta} \cdot \boldsymbol{g}_\psi - \frac{\cos\vartheta . \cos\varphi}{\sin\vartheta} \cdot \boldsymbol{g}_\varphi \\ \boldsymbol{k}_z &= \boldsymbol{g}_\varphi. \end{aligned}$$

In the following we use the abbreviations:

(4) (5) $$\mathbf{f}_i = \sum_\lambda p_i^\lambda \cdot \mathbf{g}_\lambda; \quad \mathbf{k}_i = \sum_\lambda q_i^\lambda \cdot \mathbf{g}_\lambda$$

(6A, B) $$\mathbf{g}_\lambda = \sum_i p_{i\lambda}\mathbf{f}_i = \sum_i q_{i\lambda}\mathbf{k}_i$$

For the angle of rotation about $\mathbf{f}_i$ resp. $\mathbf{k}_i$, belonging to a rotation defined by $d\vartheta^\lambda$ we have:

(7) (8) $$\delta\omega_i = \sum_\lambda p_{i\lambda} d\vartheta^\lambda \text{ resp. } \delta\omega_i = \sum_\lambda q_{i\lambda} d\vartheta^\lambda$$

For $\vartheta = 0$ (2) and (3) cannot be used. This is connected with the fact that the Eulerian angles are discontinuous in the neighbourhood of the normal position.

7. Motion. Angular velocity.

„A body is in motion" means: the position changes continuously with the time. The position is determined by a rotation from the normal position; a motion can accordingly be described as a sequence of rotations, depending continuously on the time, $R(t)$. The matrix describing the position is given by $K(t)_{mn} = (\mathbf{f}_m \cdot \mathbf{k}(t)_n)$.

If the body is not only rotating but if also the centre is moving, what we have said will still hold for the orientation. To describe the total motion we must also give the coordinates of the centre as functions of the time.

To such a sequence of rotations corresponds a continuous curve in the "space" of the parameters ξ, η, ζ, χ.

The orientation at the time $t + \Delta t$ is obtained from that at the time t by the rotation $R(t + \Delta t) \cdot R(t)^{-1}$. Let Δt grow smaller and smaller. The transformation will be determined by a vector $\Delta t \cdot \mathbf{p}$ and we will have:

$$\mathbf{r}(t + \Delta t) - \mathbf{r}(t) = \Delta t[\mathbf{p} \times \mathbf{r}]$$

or

(1) $$\dot{\mathbf{r}} = [\mathbf{p} \times \mathbf{r}].$$

The vector $\mathbf{p}$ is called *angular velocity*.

From [6,2 (7), (8)] follows at once the connection between the

components of $\mathbf{p}$ in the $\mathbf{k}$- and $\mathbf{f}$-system — we call them q_i and p_i respectively — and the time-derivatives $\dot{\vartheta}^\nu$. We have:

(2) (3) $$p_i = \sum p_{i\lambda}\dot{\vartheta}^\lambda; \qquad q_i = \sum q_{i\lambda}\dot{\vartheta}^\lambda$$

and:

(4) (5) $$\dot{\vartheta}^\lambda = \sum p_i^\lambda p_i; \qquad \dot{\vartheta}^\lambda = \sum q_i^\lambda q_i.$$

B. DYNAMICS.

8. Equations of motion for a point system.

For a "material point" (that is for a particle so small that the measurement of coordinates has an inaccuracy larger then the dimensions of the particle) of mass m the equations of motion are in a system of reference that is at rest:

(1) $$m\ddot{\mathbf{r}} = \mathbf{K}$$

where $\mathbf{K}$ is the resultant of the external forces acting on the particle. If we introduce a new system of coordinates, parallel to the old one, the position of the origin being given by a vector $\mathbf{a}$, which is an arbitrary function of the time, we have:

$$\mathbf{r}' = \mathbf{r} - \mathbf{a}; \qquad \ddot{\mathbf{r}}' = \ddot{\mathbf{r}} - \ddot{\mathbf{a}}$$

(2) $$m\ddot{\mathbf{r}}' = \mathbf{K} - m\ddot{\mathbf{a}}$$

the equations of motion keep the same form but there is an additional force.

We now consider a system of n material points. Between each two of them may act forces, satisfying the following conditions:

a. they have the direction of the line connecting the two particles;

b. action = reaction.

In equations: the force $\mathbf{K}_{ik}$ with which the i^{th} particle acts on the k^{th} one, is given by $\mathbf{K}_{ik} = f_{ik}(\mathbf{r}_i - \mathbf{r}_k)$ where f_{ik} is a scalar, symmetric in i en k. Let further $\mathbf{K}_i$ be the external force acting on the i^{th} particle. We then have:

(3) $$m_i\ddot{\mathbf{r}}_i = \sum_k f_{ik}(\mathbf{r}_k - \mathbf{r}_i) + \mathbf{K}_i.$$

Summation over all points gives:

(4) $$\sum_i m_i \ddot{\boldsymbol{r}}_i = \sum_i \boldsymbol{K}_i.$$

We define: $$\sum_i m_i = \mathrm{M}; \quad \sum_i m_i \boldsymbol{r}_i = \mathrm{M}\boldsymbol{z};$$

then:

(5) $$\mathrm{M}\ddot{\boldsymbol{z}} = \sum_i \boldsymbol{K}_i.$$

One calls the point defined by $\boldsymbol{z}$ *centre of gravity*. For the centre of gravity of a system of material points the same equations hold as for a material point.

Vectorial multiplication of (3) by $\boldsymbol{r}_i$ and summation gives:

(6) $$\sum_i m_i[\boldsymbol{r}_i \times \ddot{\boldsymbol{r}}_i] = \sum_i [\boldsymbol{r}_i \times \boldsymbol{K}_i].$$

$\boldsymbol{P} = \sum_i m_i[\boldsymbol{r}_i \times \dot{\boldsymbol{r}}_i]$ is called the (resultant) *angular momentum.* $\boldsymbol{M} = \sum_i [\boldsymbol{r}_i \times \boldsymbol{K}_i]$ the resultant *moment of the external forces;* (6) now becomes:

(7) $$\dot{\boldsymbol{P}} = \boldsymbol{M}.$$

We introduce a new coordinate system with the origin in the centre of gravity and the axes parallel to the old ones: $\boldsymbol{r} = \boldsymbol{z} + \boldsymbol{r}'$. Equation (7) becomes:

(8) $$\dot{\boldsymbol{P}}' = \boldsymbol{M}' + \boldsymbol{N}'$$

with:

$$\boldsymbol{P}' = \sum_i m_i[\boldsymbol{r}_i' \times \dot{\boldsymbol{r}}_i']; \quad \boldsymbol{M}' = \sum_i [\boldsymbol{r}_i' \times \boldsymbol{K}_i];$$

$\boldsymbol{N}'$ is the moment of the additional forces:

(9) $$\boldsymbol{N}' = -\sum_i [\boldsymbol{r}_i' \times m_i \ddot{\boldsymbol{z}}] = [(\sum_i m_i \boldsymbol{r}_i') \times \ddot{\boldsymbol{z}}] = 0.$$

Also in the moving system we have:

(7′) $$\dot{\boldsymbol{P}}' = \boldsymbol{M}'.$$

Further we find:

(10) $$\boldsymbol{P} = \boldsymbol{P}' + \mathrm{M} \,.\, [\boldsymbol{z} \times \dot{\boldsymbol{z}}],$$

(11) $$\boldsymbol{M} = \boldsymbol{M}' + [\boldsymbol{z} \times (\sum_i \boldsymbol{K}_i)]$$

and for the kinetic energy:

(12) $$T = \tfrac{1}{2} \sum_i m_i \dot{\boldsymbol{r}}_i^2 = \tfrac{1}{2} \sum_i m_i \dot{\boldsymbol{r}}_i'^2 + \tfrac{1}{2} \mathrm{M} \,.\, \dot{\boldsymbol{z}}^2.$$

8,1. Application to a rigid body.

We want to apply the results of [8] to a rigid body, replacing the summations by integrations and determining the velocity of each element of volume by [7 (1)]. But we do not know a priori whether this is legitimate. Of course one can from a mathematical point of view define a rigid body as a system of points between which there act certain forces, satisfying the conditions of the preceding paragraph and also, that the relative distances remain the same; but has the motion of this mathematical abstraction anything to do with the motion of real bodies? It would be absurd to try to settle this question by referring to the atomic constitution of matter: we know that the elementary particles do not obey the ordinary laws of classical mechanics; moreover they are in a state of most violent motion. We have to fall back upon experiments; the knowledge gathered from experiments with Atwoods machine or similar devices, operating with "material points", is not sufficiant for a foundation of classical mechanics.

For an axiomatic mind the problem arises: in which way may classical mechanics be deduced from the least possible number of experimental facts? But this does not interest us at present.

9. Fundamental equations for a rigid body.

The equations [8 (5)] and [8 (7′)] are just sufficient to determine the motion of a rigid body. The equations $\mathrm{M}\ddot{\boldsymbol{z}} = \sum_i \boldsymbol{K}_i$ determine the motion of the centre of gravity; the equations $\dot{\boldsymbol{P}}' = \boldsymbol{M}'$ the rotation about the centre of gravity. They have just the same

form as if the centre of gravity were at rest: the translations have no influence on the rotations.

The first problem is to express $\boldsymbol{P}$ (we omit for convenience the dashes, all our equations hold in the coordinate system with origin in the centre of gravity) in terms of the angular velocity. We have:

$$\dot{\boldsymbol{r}} = [\boldsymbol{p} \times \boldsymbol{r}]$$

$$[\boldsymbol{r} \times \dot{\boldsymbol{r}}] = [\boldsymbol{r} \times [\boldsymbol{p} \times \boldsymbol{r}]] = \boldsymbol{p}(\boldsymbol{r} \,.\, \boldsymbol{r}) - (\boldsymbol{p} \,.\, \boldsymbol{r})\boldsymbol{r}.$$

Multiplication by $\varrho d\tau$ (ϱ density, $d\tau$ element of volume) and integration gives:

$$\boldsymbol{P} = \boldsymbol{p} \,.\, \int \varrho(\boldsymbol{r} \,.\, \boldsymbol{r}) d\tau - \int \varrho \boldsymbol{r} (\boldsymbol{p} \,.\, \boldsymbol{r}) d\tau. \tag{1}$$

If we define:

$$B_{ik} = \delta_{ik} \,.\, \int \varrho(x^2 + y^2 + z^2) d\tau - \int \varrho x_i x_k d\tau \tag{2}$$

(where the x_i are supposed to be coordinates in the $\boldsymbol{f}$-system) this gives for P_i (the components in the $\boldsymbol{f}$-system):

$$P_i = \sum_k B_{ik} p_k. \tag{3}$$

Of course we can also write down (1) in the $\boldsymbol{k}$-system:

$$Q_i = \sum_k A_{ik} q_k.$$

The A_{ik} depend only on the distribution of mass in the $\boldsymbol{k}$-system, not on the orientation. Therefore they do not change during the motion. We will in the following always assume that the $\boldsymbol{k}$-system is chosen in such a way that $A_{ik} = A_i \delta_{ik}$. The coordinate axes are them the principal axes of the ellipsoid $\frac{1}{2} \sum A_{ik} x^i x^k = 1$. We now have:

$$A_i q_i = Q_i. \tag{5}$$

For the kinetic energy (as far as it depends on the rotation) we find:

$$\begin{aligned} T &= \tfrac{1}{2} \int ([\boldsymbol{p} \times \boldsymbol{r}] \,.\, [\boldsymbol{p} \times \boldsymbol{r}]) \varrho d\tau = \tfrac{1}{2} \int ([\boldsymbol{r} \times [\boldsymbol{p} \times \boldsymbol{r}]] \,.\, \boldsymbol{p}) \varrho d\tau = \\ &= \tfrac{1}{2} \sum_i Q_i q_i = \tfrac{1}{2} \sum_i P_i p_i = \tfrac{1}{2} \sum_{i,k} B_{ik} p_i p_k \\ &= \tfrac{1}{2} \sum_i A_i q_i^2 = \tfrac{1}{2} \sum_i \frac{1}{A_i} Q_i^2. \end{aligned} \tag{6}$$

10. Relative time-derivative of a vector.

If the components of a variable vector $\boldsymbol{v}$ in the $\boldsymbol{k}$-system are given by $w_i(t)$ we call the *relative time-derivative* $(\dot{\boldsymbol{v}})_{rel.}$ the vector $\sum_i \dot{w}_i(t) \boldsymbol{k}_i$. For the radius vector of any point of the body we have for example $(\dot{\boldsymbol{r}})_{rel.} = 0$. But $\dot{\boldsymbol{r}} = [\boldsymbol{p} \times \boldsymbol{r}]$. For an arbitrary vector the total change during the time dt is the sum of the "relative change" and the change because of the rotation of the $\boldsymbol{k}$-system:

$$\dot{\boldsymbol{r}} = (\dot{\boldsymbol{r}})_{rel.} + [\boldsymbol{p} \times \boldsymbol{r}]. \tag{1}$$

10,1. Eulers equations.

If we apply [10 (1)] to the equation $\dot{\boldsymbol{P}} = \boldsymbol{M}$ we get:

$$(\dot{\boldsymbol{P}})_{rel.} + [\boldsymbol{p} \times \boldsymbol{P}] = \boldsymbol{M}. \tag{2}$$

In the $\boldsymbol{k}$-system this becomes

$$\begin{aligned} \dot{Q}_1 + Q_2 Q_3 \left(\frac{1}{A_2} - \frac{1}{A_3}\right) &= M_1 \\ \dot{Q}_2 + Q_3 Q_1 \left(\frac{1}{A_3} - \frac{1}{A_1}\right) &= M_2 \\ \dot{Q}_3 + Q_1 Q_2 \left(\frac{1}{A_1} - \frac{1}{A_2}\right) &= M_3. \end{aligned} \tag{3}$$

That are the Eulerian equations. Once they are integrated one can find the Eulerian angles as functions of the time by one more integration.

To obtain a formula for the change of the K_{nm} we observe:

$$0 = \dot{\boldsymbol{f}}_i = (\dot{\boldsymbol{f}}_i)_{rel.} + [\boldsymbol{p} \times \boldsymbol{f}_i]. \tag{4}$$

In the $\boldsymbol{k}$-system this gets:

$$\dot{K}_{i1} = \frac{1}{A_3} \,.\, Q_3 K_{i2} - \frac{1}{A_2} \,.\, Q_2 K_{i3} \tag{5}$$

and so on.

11. Canonical equations.

Consider a system consisting of n particles. We introduce the following notations: x^1, x^2, x^3 are the x, y, z coordinates of the

first particle; x^4, x^5, x^6 of the second particle etc.; $m_1 = m_2 = m_3 =$ mass of first particle, $m_4 = m_5 = m_6 =$ mass of second particle and so on.
The equations of motion are:

(1) $$m_i \ddot{x}_i = K_i.$$

The kinetic energy is given by:

(2) $$T = \tfrac{1}{2} \sum_{i=1}^{3n} m_i \dot{x}_i^2 = \tfrac{1}{2} m_i \delta_{ik} \dot{x}^i \dot{x}^k$$

(we omit the sign of summation).
We define:

3) $$p_i = \frac{\partial T}{\partial \dot{x}^i} = m_i \delta_{ik} \dot{x}^k.$$

T may be expressed in terms of the p_i:

(4) $$T = \tfrac{1}{2} \cdot \frac{1}{m_i} \cdot \delta^{ik} p_i p_k$$

(1) is equivalent to:

(5a) (5b) $$\dot{x}^i = \frac{\partial T(p_k)}{\partial p_i}; \quad \dot{p}_i = +K_i.$$

This seems a useless, complicated way of writing (2). The advantage will appear if we introduce new coordinates that are arbitrary functions of the old ones, $q^\lambda(x^i)$. We then have:

(6) $$dq^\lambda = P_i^\lambda \cdot dx^i \text{ with } P_i^\lambda = \frac{\partial q^\lambda}{\partial x^i}; \quad \dot{q}^\lambda = P_i^\lambda \cdot \dot{x}^i;$$
$$dx^i = Q_\lambda^i \cdot dq^\lambda; \; Q_\lambda^i \cdot P_j^\lambda = \delta_j^i, \; Q_\lambda^i \cdot P_i^\mu = \delta_\lambda^\mu; \; \dot{x}^i = Q_\lambda^i \cdot \dot{q}^\lambda.$$

This gives:

(7) $$T = \tfrac{1}{2} m_i \delta_{ik} \cdot Q_\lambda^i \dot{q}^\lambda \cdot Q_\mu^k \dot{q}^\mu = \tfrac{1}{2} T_{\lambda\mu} \cdot \dot{q}^\lambda \dot{q}^\mu.$$

(8) $$T_{\lambda\mu} = T_{\mu\lambda}.$$

Again we define:

(9) $$p_\lambda = \frac{\partial T}{\partial \dot{q}^\lambda} = T_{\lambda\mu} \cdot \dot{q}^\mu = m_i \delta_{ik} Q_\lambda^i Q_\mu^k \cdot \dot{q}^\mu = Q_\lambda^i \cdot p_i.$$

It follows:

(10) $$\dot{q}^\mu = T^{\mu\lambda} \cdot p_\lambda \text{ with } T^{\mu\lambda} = P_i^\mu P_k^\lambda \cdot \frac{1}{m_k} \delta^{ik};$$
$$T^{\mu\lambda} \cdot T_{\lambda\nu} = \delta_\nu^\mu.$$

For $T(p_\lambda)$ we find:

(11) $$T = \tfrac{1}{2} T_{\lambda\mu} \cdot T^{\mu\varrho} p_\varrho \cdot T^{\lambda\sigma} p_\sigma = \tfrac{1}{2} T^{\varrho\sigma} p_\varrho p_\sigma.$$

Thus we have again:

(12) $$\dot{q}^\mu = \frac{\partial T(p, q)}{\partial p_\mu}.$$

Further one finds:

(13) $$\dot{p}_\lambda = \dot{Q}_\lambda^i \dot{p}_i + \dot{Q}_\lambda^i p_i = Q_\lambda^i K_i + \dot{Q}_\lambda^i p_i = K_\lambda + \dot{Q}_\lambda^i P_i^\mu p_\mu.$$

(14) $$\dot{Q}_\lambda^i P_i^\mu = - \dot{P}_i^\mu Q_\lambda^i$$

since:

$$\frac{d}{dt}\left(Q_\lambda^i P_i^\mu\right) = \frac{d}{dt}\left(\delta_\lambda^\mu\right) = 0.$$

(15) $$\frac{d}{dt}(P_i^\mu) = \frac{d}{dt}\left(\frac{\partial q^\mu}{\partial x^i}\right) = \frac{\partial}{\partial x^m}\left(\frac{\partial q^\mu}{\partial x^i}\right) \cdot \dot{x}^m = \frac{\partial}{\partial x^i}(P_m^\mu) \cdot \frac{\delta^{ms}}{m^s} p^s.$$

Accordingly:

$$\dot{Q}_\lambda^i p^i = - Q_\lambda^i \frac{\partial}{\partial x^i}(P_m^\mu) \cdot \frac{\delta^{ms}}{m_s} p_s p_\mu =$$

(16) $$= - \frac{\partial}{\partial q^\lambda}(P_m^\mu) \cdot \frac{\delta^{ms}}{m_s} \cdot P_s^\varrho \, p_\varrho p_\mu = - \frac{\partial}{\partial q^\lambda}(T).$$

The equations of motion are:

(17a) (17b) $$\dot{q}^\mu = \frac{\partial T}{\partial p_\mu}; \quad \dot{p}_\mu = - \frac{\partial T}{\partial q^\mu} + K_\mu.$$

In many cases we will have:

$$K_i = - \frac{\partial V}{\partial x^i},$$

where V is the potential energy. We then have:

(19) $$K_\lambda = -\frac{\partial V}{\partial q^\lambda}$$

and, calling T + V = H:

(20a) (20b) $$\dot{q}^\mu = \frac{\partial H}{\partial p_\mu}; \quad \dot{p}_\mu = -\frac{\partial H}{\partial q^\mu}.$$

We call (20) the *canonical equations;* the function $H(p, q)$ is called the *Hamiltonian* for our system. From our deduction it follows, that the canonical equations are invariant under an arbitrary transformation of coordinates. (As a matter of fact they are invariant under a much more general class of transformations).

11, 1. Application to a rigid body.
We will again assume that a rigid body may be treated as a system of points between which there act certain forces, that make the distances between all points remain the same. Further we will assume that there are no external forces. In stead of the rectangular coordinates we will introduce: the coordinates of the centre of gravity c_1, c_2, c_3; the Eulerian angles ϑ^ν for a $\boldsymbol{k}$-system with origin the centre of gravity (we may again choose the principal axes of the tensor of inertia as $\boldsymbol{k}$-axes) and some coordinates ξ_ϱ determining the relative distances. When the forces are of the form $f_{ik}(\boldsymbol{r}_i - \boldsymbol{r}_k)$, (see [8]), we will have:

(1a) (1b) $$K_{c^i} = 0, \quad K_{\vartheta^\nu} = 0;$$

for it is easy to see that the expression $K_i \delta x^i$ (where K_1, K_2, K_3 are the x, y, z component of the resultant of the internal forces acting on the first point, and so on) vanishes for all variations δx^i that do not change the relative distances. Now:

(2) $$K_i \delta x^i = K_{c^i} \delta c^i + K_\nu \delta \vartheta^\nu + K_\varrho \delta \xi^\varrho$$

and this can only vanish for arbitrary δc^i, $\delta \vartheta^\nu$ — $\delta \xi^\varrho$ being zero — if $K_{c^i} = K_\nu = 0$.

As we assume that $\dot{\xi}^\varrho = 0$ during the motion we have only to calculate T as function of the $\dot{c}^i$ and $\dot{\vartheta}^\nu$ and apply [11 (17)]. One finds, using [8 (12), [9 (6)], [7 (2), (3)]:

(3) $$\begin{aligned} T &= \tfrac{1}{2} M \sum \dot{c}_i^2 + \tfrac{1}{2} \sum_{i,k} B_{ik} p_{i\lambda} p_{k\mu} \dot{\vartheta}^\lambda \dot{\vartheta}^\mu = \\ &= \tfrac{1}{2} M \sum \dot{c}_i^2 + \tfrac{1}{2} \sum_i A_i q_{i\lambda} q_{i\mu} \dot{\vartheta}^\lambda \dot{\vartheta}^\mu. \end{aligned}$$

For c_i and p_{c_i} we find the ordinary equations for a point of mass M. Further one finds:

(8) $$\frac{\partial T}{\partial \dot{\vartheta}^\mu} = \pi_\mu = \sum_{i,k} B_{ik} p_{i\lambda} p_{k\mu} \dot{\vartheta}^\lambda = \sum_i A_i q_{i\lambda} q_{i\mu} \dot{\vartheta}^\lambda$$

(9) $$P_i = \sum_k B_{ik} p_{k\lambda} \dot{\vartheta}^\lambda$$

(10) $$Q_i = A_i q_{i\lambda} \dot{\vartheta}^\lambda$$

(11) $$\pi_\mu = \sum_k p_{k\mu} P_k = \sum_k q_{k\mu} Q_k.$$

If there are external forces we have to calculate the potential energy as function of the c_i and ϑ^ν and add it to T.

12. Infinitesimal canonical transformations.
Consider a transformation:

(1a) $$q^{*\nu} = q^\nu + \varepsilon \frac{\partial f(q, p)}{\partial p_\nu}$$

(1b) $$p^*_\nu = p_\nu - \varepsilon \frac{\partial f(q, p)}{\partial q^\nu}$$

where f is an arbitrary function of the p and q, ε an infinitesimal constant. We will interpret it as a change of coordinates in the p, q "space": a point that before the transformation has the coordinates p_ν, q^λ is called p^*_ν, $q^{*\lambda}$ after the transformation. This transformation is canonical: p^*, q^* satisfy equations of the canonical type. One finds (observing that in terms multiplied by ε the difference between p and p^*, q and q^* can be neglected):

$$\dot{q}^{*\nu} = \dot{q}^{\nu} + \varepsilon \frac{\partial}{\partial q^{\nu}}\left(\frac{\partial f(q,p)}{\partial p_{\nu}}\right)\dot{q}^{\lambda} + \varepsilon \frac{\partial}{\partial p^{\lambda}}\left(\frac{\partial f(q,p)}{\partial p_{\nu}}\right)p_{\nu} =$$

$$= \frac{\partial}{\partial p^{*\lambda}}\left(\mathrm{H}(q^* - \varepsilon\frac{\partial f}{\partial p},\ p^* + \varepsilon\frac{\partial f}{\partial q})\right)\cdot\frac{\partial p^{*}{}_{\lambda}}{\partial p_{\nu}} +$$

$$+ \frac{\partial}{\partial q^{*}{}_{\lambda}}\left(\mathrm{H}(q^* - \varepsilon\frac{\partial f}{\partial p},\ p^* + \varepsilon\frac{\partial f}{\partial p})\right)\cdot\frac{\partial q^{*\lambda}}{\partial p_{\nu}} +$$

$$+ \varepsilon\left(\frac{\partial^2 f}{\partial q^{\lambda}\partial p_{\nu}}\cdot\frac{\partial \mathrm{H}}{\partial p_{\lambda}} - \frac{\partial^2 f}{\partial p_{\lambda}\partial p_{\nu}}\cdot\frac{\partial \mathrm{H}}{\partial q^{\lambda}}\right) =$$

$$= \frac{\partial}{\partial p^{*}_{\nu}}\left(\mathrm{H}(q^*, p^*) - \varepsilon\frac{\partial \mathrm{H}(^*)}{\partial q^{*\lambda}}\cdot\frac{\partial f(^*)}{\partial p^{*}{}_{\lambda}} + \varepsilon\frac{\partial \mathrm{H}(^*)}{\partial p^{*}{}_{\lambda}}\cdot\frac{\partial f(^*)}{\partial q^{*\lambda}}\right) =$$

(2) $$= \frac{\partial}{\partial p^{*}_{\nu}}\left(\mathrm{H}^*(q^*, p^*)\right).$$

In the same way:

(3) $$\dot{p}^{*}_{\nu} = -\frac{\partial}{\partial q^{*\nu}}\left(\mathrm{H}^*(p^*,\ q^*)\right).$$

We may say that $\mathrm{H}^{*}_{(*)}$ is the old Hamiltonian expressed in terms of the new variables: it is obtained by substituting in $\mathrm{H}(q,\ p)$ for q and p their expressions as functions of q^*, p^*.

12, 1. Poisson Brackets.

One calls Poisson Bracket (P. B) of two functions f, g the expression:

(1) $$(f,\ g) = \left(\frac{\partial f}{\partial q^{\nu}}\cdot\frac{\partial g}{\partial p_{\nu}} - \frac{\partial f}{\partial p_{\nu}}\cdot\frac{\partial g}{\partial q^{\nu}}\right),$$

From this definition one deduces:

(2) $$(f,\ g) = -\,(g,\ f).$$

(3) $$(f + g,\ h) = (f,\ h) + (g,\ h).$$

(4) $$(fg,\ h) = f(g,\ h) + g(f,\ h).$$

(5) $$(f,\ (g,\ h)) + (g,\ (h,\ f)) + (h,\ (f,\ g)) = 0.$$

Using this notation we find for the transformed Hamiltonian H^* of [12]:

(6) $$\mathrm{H}^* = \mathrm{H} + \varepsilon(f,\ \mathrm{H}).$$

More general: let g be an arbitrary function of p and q. We define as transformed function g^* the function with the property:

(7) $$g^*(p^*,\ q^*) = g(p,\ q);$$

when the transformation $p,\ q \to p^*,\ q^*$ is given by [12 (1)] we find:

(8) $$g^* = g + \varepsilon(f,\ g).$$

12, 2. Invariance of the Hamiltonian and integrals.

For the time derivative of an arbitrary function f not containing the time explicitly we have:

(1) $$\frac{df}{dt} = (f,\ \mathrm{H}).$$

By comparing this with [12,1 (6)] one infers:

If a function f is an integral — that is: $\frac{df}{dt} = 0$ — then the Hamiltonian is not changed by the infinitesimal transformation generated by f.

If on the other hand we know that H is invariant under a certain transformation, we can find and integral by finding the function by which the transformation is generated. We know for example that the Hamiltonian for a rigid body in absence of external fields, will keep the same form if we rotate the ***f***-system: all directions in space are equivalent. There will accordingly exist three integrals, belonging to the infinitesimal rotations about the three axes of coordinates. We will find that these three integrals are the components of the angular momentum. The Hamiltonian will also remain the same if a translation is carried out. To the translations belong, as is easily seen, the three integrals $\mathrm{M}\dot{c}_i$.

13. The transformations generated by P_i and Q_i.

If we take in [12 (1)] for $f(pq)$, P_i resp. Q_i we find, using [11,1 (9) (10)]:

(1a) (2a) $\qquad \vartheta^{*\nu} - \vartheta^{\nu} = \varepsilon p_i^{\nu}; \qquad \vartheta^{*\nu} - \vartheta^{\nu} = \varepsilon q_i^{\nu};$

(1b) (2b) $\pi_\nu^* - \pi_\nu = -\varepsilon \frac{\partial}{\partial \vartheta^\nu}(p_i^\lambda)\pi_\lambda; \quad \pi_\nu^* - \pi_\nu = -\varepsilon \frac{\partial}{\partial \vartheta^\nu}(q_i^\lambda)\pi_\lambda.$

That means: the transformation of the Eulerian angles is a positive rotation about $\boldsymbol{f}_i$ resp. $\boldsymbol{k}_i$. But in order to know everything about the transformation, we have to know also in which way P_i and Q_i are changed. We have therefore to calculate the P. B's (Q_i, Q_k), (P_i, P_k), (Q_i, P_k). One finds:

(3) $$\left(\frac{\partial p_1^\lambda}{\partial \vartheta^\nu} \cdot p_2^\nu - \frac{\partial p_2^\lambda}{\partial \vartheta^\nu} \cdot p_1^\nu\right) = p_3^\lambda \quad \text{and so on.}$$

(4) $$\left(\frac{\partial q_1^\lambda}{\partial \vartheta^\nu} \cdot q_2^\nu - \frac{\partial q_2^\lambda}{\partial \vartheta^\nu} \cdot q_1^\nu\right) = -\, q_3^\lambda \quad \text{and so on.}$$

(5) $$\left(\frac{\partial q_k^\lambda}{\partial \vartheta^\nu} \cdot p_l^\nu - \frac{\partial p_l^\lambda}{\partial \vartheta^\nu} \cdot q_k^\nu\right) = 0 \qquad \text{for all } l,\ k.$$

Consequently:

(6) $$(P_1, P_2) = P_3.$$

(7) $$(P_l, Q_k) = 0.$$

(8) $$(Q_1, Q_2) = -\, Q_3.$$

For the rotation generated by εQ_2 this gives:

(9a) $$Q_1^*(\vartheta^*, \pi^*) = Q_1(*) + \varepsilon\, Q_3(*) = Q_1\,(\vartheta, \pi).$$

(9b) $$Q_3^*(*) = -\,\varepsilon\, Q_1(*) + Q_3(*) = Q_3(\vartheta, \pi).$$

(9c) $$Q_2^*(*) = Q_2(*) = Q_2(\vartheta, \pi).$$

(9d) $$P_i^* = P_i \qquad \text{for all } i.$$

For the rotation generated by εP_2:

(10a) $$P_1^* = P_1 - \varepsilon P_3.$$

(10b) $$P_3^* = \varepsilon P_1 + P_3.$$

(10c) $$P_2^* = P_2.$$

(10d) $$Q_i^* = Q_i.$$

To make things look nicer, we will for one moment deviate from the rule that all transformations are transformations of coordinates.
(Of course what we say may at once be translated into transformation-of-coordinate-language).

P_i generates a rotation about $\boldsymbol{f}_i$ of the body together with its angular momentum.

Q_i generates a rotation of the body about $\boldsymbol{k}_i$ but the angular momentum keeps the same position in space.

Only from (1a), (2a) follows already:

(11) $$(P_1, K_{2k}) = (K_{1k}, P_2) = K_{3k} \quad \text{and so on for all } k,$$

(12) $$(Q_1, K_{2k}) = (K_{k1}, Q_2) = -\, K_{k3} \quad \text{and so on for all } k.$$

For the K_{lm} are functions of ϑ^ν only, and it follows from their geometrical meaning:

(13) $$\| K(\vartheta^\nu + \varepsilon^i p_i^\nu)_{nm} \| = \| 1 + \varepsilon^i D_i \| \, \| K(\vartheta^\nu)_{nm} \|$$

(14) $$\| K(\vartheta^\nu + \varepsilon^i q_i^\nu)_{nm} \| = \| K(\vartheta^\nu)_{nm} \| \, \| 1 + \varepsilon^i D_i \|$$

For a rotation about $\boldsymbol{f}_2$ this gives for instance:

(15a) $$K^*(\vartheta^*)_{1k} = K(\vartheta)_{1k} = K(\vartheta^*)_{1k} - \varepsilon K(\vartheta^*)_{3k}$$

(15b) $$K^*(\vartheta^*)_{3k} = K(\vartheta)_{3k} = \varepsilon K(\vartheta^*)_{1k} + K(\vartheta^*)_{3k}$$

(15c) $$K^*_{2k} = K_{2k};$$

similar relations hold for the other rotations. This leads at once to (11) and (12).

From (6) and (11) together with $P_i = \sum_k K_{ik} Q_k$ the other P. B's may be deduced, using the rules [12, 1 (2) — (5)] and the orthogonality relations for the K_{ik} only.

13, 1. General relation between angular momentum and rotations.

The connection between angular momentum and rotations is of a much more general nature, than the somewhat laborious evaluations of P . B's would suggest.

Consider a point system. Then:

(1) $$\boldsymbol{P} = \sum m_i [\boldsymbol{r}_i \times \dot{\boldsymbol{r}}_i]$$

($\boldsymbol{r}_1$ radius vector of first particle, $\boldsymbol{r}_2$ of second particle; m_1 mass of first particle, m_2 mass of second particle and so on).

$$P_y = \sum_i (z_i p_{x_i} - x_i p_{z_i})$$

generates the transformation:

(2a) $$x_i^* - x_i = \varepsilon z_i, \qquad p_{x_i}^* - p_{x_i} = \varepsilon p_{z_i},$$

(2b) $$z_i^* - z_i = -\varepsilon x_i, \qquad p_{z_i}^* - p_{z_i} = -\varepsilon p_{x_i},$$

(2c) $$y_i^* - y_i = 0, \qquad p_{y_i}^* - p_{y_i} = 0;$$

a rotation of the coordinate system.

Not only for x_i, y_i, z_i; p_{x_i}, p_{y_i}, p_{z_i} but for every vector $\boldsymbol{V}$ the components of which are functions of x_i, p_{x_i} we have;

(3a) $$V_1^*(x^*, p^*) = V_1(x, p) = V_1(x^*, p^*) - \varepsilon V_3(x^*, p^*),$$

(3b) $$V_3^*(x^*, p^*) = V_3(x, p) = \varepsilon V_1(x^*, p^*) + V_3(x^*, p^*),$$

(3c) $$V_2^*(x^*, p^*) = V_2(x, p) = V_2(x^*, p^*)$$

and accordingly:

(4) $$(P_2, V_1) = -V_3.$$

In particular:

(5) $$(P_1, P_2) = P_3.$$

If one introduces new coordinates the same relations will hold for the P . B's of P_i, V_i expressed in terms of the new variables; for the P . B's are invariant under an arbitrary change of coordinates.

As a matter of fact they are invariant under any canonical transformation; this may easily be verified for an infinitesimal

transformation. If $p = (v, w)$ and the transformation is generated by f we have:

(6) $$p^* = p + \varepsilon(f, p) = p + \varepsilon(v, (f, w)) + \varepsilon((f, v), w) = (v^*, w^*).$$

Now classical mechanics are based on the assumption, that any system can be described as a system of points between which there act certain forces, that make certain functions of the coordinates remain constant. Consequently the relations (4) (5) hold for any holonomic system.

In the case of the rigid body the relations [13 (6) (11)] (and therefore all the P . B relations) may thus be written down at once, without even knowing in which way the quantities P_i, Q_k, K_{ik} depend on the Eulerian angles.

Another consequence of the connection between angular momentum and infinitesimal rotations is: for any system moving in empty space, the components of angular momentum will be integrals. For the Hamiltonian will not change, if a rotation is carried out.

14. P . B's and equations of motion.

We have deduced the following relations:

(1) $$(P_1, P_2) = P_3.$$

(2) $$(P_i, Q_k) = 0.$$

(3) $$(Q_1, Q_2) = -Q_3$$

(4) $$(P_1, K_{2k}) = (K_{1k}, P_2) = +K_{3k}.$$

(5) $$(Q_1, K_{k2}) = (K_{k1}, Q_2) = -K_{k3}.$$

The Hamiltonian is given by:

(6) $$H = \tfrac{1}{2} \sum_i \frac{Q_i^2}{A_i}.$$

Applying the equation:

(7) $$\dot{f} = (f, H)$$

and using the rules [12, 1 (2)—(5)] we find:

(8) $$\dot{P}_i = (P_i,\ H),$$

(9) $$\dot{Q}_1 = \tfrac{1}{2}\left(Q_1,\ \frac{Q_1^2}{A_1}+\frac{Q_2^2}{A_2}+\frac{Q_3^2}{A_3}\right) = -\,Q_2Q_3\left(\frac{1}{A_2}-\frac{1}{A_3}\right),$$

(10) $$\dot{K}_{k1} = \tfrac{1}{2}\left(K_{k1},\ \frac{Q_1^2}{A_1}+\frac{Q_2^2}{A_2}+\frac{Q_3^2}{A_3}\right) = -\frac{Q_2}{A_2}\,.\,K_{k3}+\frac{Q_3}{A_3}\,.\,K_{k2};$$

the equations of [10, 1].

II.

QUANTUM THEORY OF THE RIGID BODY.

1. Introduction.

In classical mechanics it was possible, starting from the equations of motion for a "point" and using some simple axioms based on experimental facts [I 8, 1], to arrive at equations of motion for a large variety of systems.

Quantum mechanics has brought a new set of equations, describing the behaviour of the elementary particles — electrons and nuclei. Moreover the forces of interaction between these particles are known to be given by the Coulomb law of interaction. Consequently every problem in quantum mechanics has to be a problem of more bodies; for supplementary axioms there is no room.

The possibility exists that, in treating the motion of certain systems containing several nuclei and electrons (a molecule), it will be permitted — with a certain degree of approximation perhaps — to treat the *internal* motion and the motion of the system as a whole ("*external motion*") as independent phenomena. For this external motion one would then expect to find equations, having a certain analogy to the classical equations for a rigid body. Whether such a treatment is possible must be deduced from the fundamental equations.

When we in this chapter build up a quantum theory of the rigid body on the assumption that external and internal motion may be treated as independent, we must not forget that it is a mere hypothesis to assume that this theory has anything to do with reality. And though this chapter may contain nice

examples, illustrating the mathematical methods of quantum mechanics, its physical interest is but small, until the legitimacy of our treatment is proved or in any case made plausible from physical arguments.

2. The Schrödinger equation.

The Schrödinger equation for a system of many particles is:

$$(1) \qquad -h^2 \cdot \sum_i \frac{1}{2m_i} \Delta_i \varphi + V\varphi = -\frac{h}{i}\frac{\partial \varphi}{\partial t}$$

or abbreviating:

$$(2) \qquad \mathcal{S}_x\, \varphi = -\frac{h}{i}\frac{\partial \varphi}{\partial t}.$$

(Notation: m_i = mass of i^{th} particle;

$$\Delta_i = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2},$$

x_i, y_i, z_i coordinates of i^{th} particle;
h = Planck's constant / 2π;
V = potential energy as function of x_i, y_i, z_i).

The stationary energy levels are found by substituting:

$$(3) \qquad \varphi = e^{-\frac{i}{h}Et} \cdot \psi$$

and seeking those values of E (*eigenvalues*) for which the resulting equation:

$$(4) \qquad \mathcal{S}_x \psi = E\psi,$$

has a onevalued, quadratically integrable solution (*eigenfunction*).

The eigenfunctions form a complete orthogonal set. We will in the following always assume that they are normalized:

$$(5) \qquad \int \bar{\psi}\psi dV = 1;$$

($dV = dx_1 dy_1 dz_1 \cdot dx_2 dy_2 dz_2 \ldots$; the integration must be performed over all x_i, y_i, z_i from $-\infty$ to $+\infty$).

2, 1. Introduction of new coordinates.

If we introduce new coordinates q^λ such that the "lineelement", that was first given by:

$$(1) \qquad ds^2 = \sum_i m_i(dx_i^2 + dy_i^2 + dz_i^2),$$

becomes:

$$(2) \qquad ds^2 = g_{\lambda\mu} dq^\lambda dq^\mu,$$

[2 (1)] becomes:

$$(3) \qquad \mathcal{S}_q\, \varphi = \left[-\frac{h^2}{2}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q^\lambda}\sqrt{g} \cdot g^{\lambda\mu}\frac{\partial}{\partial q^\mu} + V\right]\varphi = -\frac{h}{i}\frac{\partial \varphi}{\partial t},$$

where $\sqrt{g} = \sqrt{\mathrm{Det}\,(g_{\lambda\mu})}$ is the "element of volume" in terms of the new variables.

We can now, just as in the case of classical mechanics, introduce as new coordinates the coordinates of the centre of gravity, c_i, the Eulerian angles ϑ^ν and "internal" coordinates ξ^ϱ. We then have:

$$(4) \qquad ds^2 = M(dc_1^2 + dc_2^2 + dc_3^2) + du^2$$

where du^2 does not contain c_i or dc_i (M = total mass). Application of (3) gives:

$$(5) \qquad \mathcal{S}_{c,\vartheta,\xi} = -\frac{h^2}{2M}\left(\frac{\partial^2}{\partial c_1^2} + \frac{\partial^2}{\partial c_2^2} + \frac{\partial^2}{\partial c_3^2}\right) + U$$

where U does not involve c_i or $\frac{\partial}{\partial c_i}$.

The eigenfunctions of $\mathcal{S}_{c,\vartheta,\xi}$ may be written as products:

$$(6) \qquad \psi_E = f(c)\chi(\vartheta, \xi)$$

where $f(c)$ is an eigenfunction satisfying:

$$(7) \qquad -\frac{h^2}{2M}\left(\frac{\partial^2}{\partial c_1^2} + \frac{\partial^2}{\partial c_2^2} + \frac{\partial^2}{\partial c_3^2}\right) f = E_1 f$$

(that is the Schrödinger equation for an elementary particle), χ an eigenfunction satisfying:

$$(8) \qquad U\chi = E_2\chi.$$

and

$$E = E_1 + E_2. \tag{9}$$

If now for a molecule du^2 would be of the form

$$du^2 = g_{\lambda\mu}(\vartheta)d\vartheta^\lambda d\vartheta^\mu + g_{\varrho\sigma}(\xi)d\xi^\varrho d\xi^\sigma, \tag{10}$$

one could, as the potential energy V depends on ξ^ϱ only, apply the same reasoning. Every eigenfunction could then be written as a product,

$$\chi(\vartheta, \xi) = u(\vartheta)v(\xi) \tag{11}$$

and $u(\vartheta)$ would be an eigenfunction satisfying:

$$\mathcal{H}u = Eu \tag{12}$$

with:

$$\mathcal{H} = -\frac{h^2}{2}\frac{1}{\sqrt{g}}\frac{\partial}{\partial\vartheta^\lambda}\sqrt{g}\, g^{\lambda\mu}\frac{\partial}{\partial\vartheta^\mu}, \tag{13}$$

where $g^{\lambda\mu}$ and $\sqrt{g}$ must be taken for the lineelement

$$g_{\lambda\mu}(\vartheta)d\vartheta^\lambda d\vartheta^\mu.$$

In this chapter we will investigate the properties of a system, the wave equation for which is supposed to be given by (13); whether the results of this "wave mechanics of the rigid body" may be applied to the external motion of real systems remains undecided.

2, 2. Form of the wave equation.

From [I 11,1 (3)] it follows that the $g_{\lambda\mu}(\vartheta)$ are given by:

$$g_{\lambda\mu} = \sum_i A_i q_{i\lambda} q_{i\mu} \tag{1}$$

and for $g^{\lambda\mu}$ we have

$$g^{\lambda\mu} = \sum_i \frac{1}{A_i} q_i^\lambda q_i^\mu. \tag{2}$$

To determine the determinant $\sqrt{g}$ we observe that the matrix $g_{\lambda\mu}$ is equal to

$$\| \tilde{q}_{i\lambda} \| \,.\, \| A_i\delta_{ik} \| \,.\, \| q_{k\mu} \|$$

(where the sign $\sim$ means that we have to interchange rows and columns). For $\sqrt{g}$ we have consequently (apart from a constant factor that does not interest us):

$$\sqrt{g} = \text{Det} \,\| q_{i\mu} \| = \text{Det} \,\| p_{i\mu} \|. \tag{3}$$

And this determinant, that is equal to the volume of the parallelopiped built up by the three vectors $\boldsymbol{g}_\vartheta$, $\boldsymbol{g}_\varphi$, $\boldsymbol{g}_\psi$ is equal to $\sin\vartheta$.

The wave equation is:

$$Eu = -\frac{h^2}{2}\sum_i \frac{1}{A_i}\left(\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta^\lambda}\sin\vartheta\, q_i^\lambda q_i^\mu \frac{\partial}{\partial\vartheta^\mu}\right)u. \tag{4}$$

We could now try to find the eigenvalues and eigenfunctions of this equation. But we will proceed along a different line. We will give another formulation of the quantum theory of the rigid body, using the methods of matrix mechanics. The matrix mechanical formulation has not only the advantage of revealing a close formal analogy to the classical theory, but it also offers a convenient way to determine all physically important quantities. Before formulating the algebraical problem we will give a short survey of the main features of the connection between wave and matrix mechanics, confining ourselves to the case of one electron.

3. Interpretation of wave mechanics.

Let the eigenfunctions of

$$-\frac{h^2}{2m}\Delta\psi + V\psi = E\psi \tag{1}$$

be called $\psi_n(x, y, z)$ and $\varphi_n = e^{-\frac{h}{i}Et} \,.\, \psi_n$.

The quantity $\varphi_n(x, y, z)\,\bar{\varphi}_n(x, y, z)$ gives the probability of finding the electron at the point x, y, z. For any function of the coordinates, f, we accordingly have: $\int\bar{\varphi}_n f\varphi_n$ is the mean value of f in the state n.

The transition probability from the state n to the state m ($E_n > E_m$) is found by calculating the emission of an electric density:

(2) $$\varrho_{nm} + \varrho_{mn} = e(\bar{\varphi}_n \varphi_m + \bar{\varphi}_m \varphi_n)$$

(e = charge of the electron) according to classical electrodynamics. The frequency of the radiation is given by:

$$\nu = \frac{E_n - E_m}{2\pi h},$$

for:

(3) $$\varrho_{nm} = e^{\frac{i}{h}(E_n - E_m)t} \cdot \underset{o}{\varrho}_{nm}$$

where

$$\underset{o}{\varrho}_{nm} = \bar{\psi}_n \psi_m$$

does not involve t.

If the wave length of the light emitted is long compared with the dimensions of the region within which the wave functions are appreciably different from zero, the emission will be determined by the dipole moment:

$$e(x_{nm} + x_{mn}) = e \int (\varrho_{nm} x + \varrho_{mn} x).$$

(5) $$x_{nm} = e^{\frac{i}{h}(E_m - E_n)t} \cdot \underset{o}{x}_{nm}$$

(6) $$\underset{o}{x}_{nm} = \int \underset{o}{\varrho}_{nm} x = \int \bar{\psi}_n x \bar{\psi}_m.$$

The total energy emitted per unit time will be:

(7) $$\tfrac{4}{3} \frac{(2\pi\nu)^4}{c^3} \{ | x_{nm} |^2 + | y_{nm} |^2 + | z_{nm} |^2 \}.$$

3,1. Operators and matrices.

(1) $$x\varphi_n = \sum_m x_{mn} \varphi_m.$$

(2) $$x\psi_n = \sum_m \underset{o}{x}_{mn} \psi_m$$

where x_{mn}, $\underset{o}{x}_{mn}$ are the quantities defined in the preceding section. To the "operator" that changes φ into $x\varphi$ corresponds a linear

transformation. The matrix of this transformation, x, is *Hermitean:* $x_{mn} = \bar{x}_{nm}$.

If to every function $f(x, y, z)$ corresponds another function f' we write symbolically $f' = \mathcal{O}f$ and call $\mathcal{O}$ an *operator.* If $\mathcal{O}(f_1 + f_2) = \mathcal{O}f_1 + \mathcal{O}f_2$ for all f_1, f_2 we call $\mathcal{O}$ a *linear operator.* To every linear operator, $\mathcal{L}$, corresponds a linear transformation (with Hermitean matrix) in φ_n space. We have:

(3) $$\mathcal{L}\varphi_n = \sum_m L_{mn} \varphi_m$$

with:

(4) $$L_{mn} = \int \varphi_m \mathcal{L} \varphi_n$$

For an arbitrary function

(5) $$f = \sum_p a_p \varphi_p$$

we have:

(6) $$\mathcal{L}f = \mathcal{L} \sum_p a_p \varphi_p = \sum_p a_p (\mathcal{L}\varphi_p) = \sum_{p,m} a_p L_{mp} \varphi_m =$$

(7) $$= \sum_m a_m^* \varphi_m$$

with

$$a_m^* = \sum_p L_{mp} a_p.$$

To the product of two operators corresponds the product of the two matrices in the same order:

(8) $$\underset{2}{\mathcal{L}} \underset{1}{\mathcal{L}} \varphi_n = \underset{2}{\mathcal{L}} \sum_m \underset{1}{L}_{mn} \varphi_n = \sum_m \underset{1}{L}_{mn} (\underset{2}{\mathcal{L}} \varphi_m) =$$

$$= \sum_{m,p} \underset{1}{L}_{mn} \underset{2}{L}_{pm} \varphi_p = \sum_{m,p} \underset{2}{L}_{pm} \underset{1}{L}_{mn} \varphi_p.$$

Consider the operator

(9) $$\frac{h}{i} \frac{\partial}{\partial x_i} = p_i$$

(x_1, x_2, $x_3 = x$, y, z).

Also here

(10) $$(p_i)_{nm} = (\bar{p}_i)_{mn}:$$

$$\int \bar{\varphi}_n \frac{\partial}{\partial x_i} \varphi_m = - \int \varphi_m \frac{\partial}{\partial x_i} \bar{\varphi}_n$$

(assuming that the wave functions vanish for $x \to \infty$).

We have:

(11) $$p_i x_k f - x_k p_i f = (p_i x_k) f = \frac{h}{i} \delta_{ik} \cdot f$$

for all f and accordingly:

(12) $$\boldsymbol{p_i x_k - x_k p_i = \frac{h}{i} \delta_{ik}}.$$

The Schrödinger operator is given by:

(13) $$\mathcal{S}_x = \frac{1}{2m} \sum p_i^2 + V(x)$$

and the equation

(14) $$\mathcal{S}_x \varphi_n = E_n \varphi_n$$

shows that the corresponding matrix:

(15) $$\boldsymbol{H = \frac{1}{2m} \sum p_i^2 + V(x)}$$

is a diagonal matrix with diagonal elements E_n.

For any operator f that does not depend on the time we have:

(16) $$f_{nm} = e^{\frac{h}{i}(E_n - E_m)t} \overset{\circ}{f}_{nm}$$

where $\overset{\circ}{f}_{nm} = \int \bar{\psi}_n f \psi_m$ is independent of the time.

(17) $$\dot{f}_{nm} = \frac{i}{h}(E_n - E_m) f_{nm}$$

and therefore:

(18) $$\boldsymbol{ih\dot{f} = fH - Hf}.$$

For $\dot{x}_i$ we find, using this relation:

$$ih\dot{x}_i = x_i \cdot \frac{1}{2m} p_i^2 - \frac{1}{2m} p_i^2 . x_i = -\frac{1}{m} \cdot \frac{h}{i} p_i$$

(19) $$\dot{x}_i = \frac{1}{m} p_i;$$

p plays the part of a momentum.

It is a natural generalization of [3] to assume, that the diagonal element of any operator that is a function of p_i and x_i is the mean value of this function. For example will

$$(x_1 p_2 - p_1 x_2)_{nn}$$

be the mean value of the z component of the angular momentum in the state n.

3, 2. Matrix mechanics.

We summarize the results of the preceding section:

There exists a set of matrices x_i, p_i, H satisfying the following conditions:

a. $x_i x_k - x_k x_i = 0$ (for all i, k),
$p_i p_k - p_k p_i = 0$ (for all i, k),
$p_i x_k - x_k p_i = \frac{h}{i} \delta_{ik}$;

b. $H = \frac{1}{2m} \sum_i p_i^2 + V(q)$;

c. all matrices are Hermitean;

d. H is a diagonal matrix;

e. $ih\dot{f} = fH - Hf$, for any matrix f, corresponding to an operator independent of t.

The diagonal elements of H are the stationary energy levels, the diagonal elements of any matrix representing a physical quantity are the mean values of this quantity for the stationary states, x_{nm} determines the transition probability.

If we can determine by algebraical methods a set of matrices x_i, p_k, H satisfying the conditions $a - e$ (e must be satisfied by any of the x_i, p_k, H) and if we can show that the solution of the algebraical problem is unique, then we have found all physically important quantities without solving the wave equation.

We may first omit e. If a set of matrices is found that satisfies $a - d$, a set of matrices also satisfying e is obtained by multiplying the nm element of all matrices by $\exp(i/h)(E_n - E_m)t$.

3, 3. Foundation of matrix mechanics.

Until now we have regarded matrix mechanics as a mathematical consequence of the wave equation. But as a matter of fact matrix mechanics was known before wave mechanics. It was

then based on arguments connected with the principle of correspondence.

The theory of dispersion had led to associating with an atom a set of quantities

$$q_{nm} e^{\frac{i}{\hbar}(E_n - E_m)t}$$

being the dipole moments that determine the transition probabilities from the state n to the state m. If we call $\boldsymbol{H}$ the matrix with elements $H_{nm} = E_n \delta_{mn}$, we at once have:

$$ih\dot{q} = \boldsymbol{qH} - \boldsymbol{Hq}. \tag{1}$$

Further for high quantum numbers q_{nm} must correspond to the o Fourier components of the classical orbits. The other laws of matrix mechanics could thus be obtained as generalizations of known results about these Fourier components.

In arriving at a definitive formulation of the theory, the formal analogy with classical mechanics offered a helpful guidance:

The expressions $\alpha(\boldsymbol{AB} - \boldsymbol{BA})$ (α an arbitrary constant) satisfy the same relations as the classical P. B's, [I 12,1 (2)—(5)]. Now (1) corresponds to the classical equation $\dot{q} = (q, H)$. We are thus led to the assumption that, whenever there exists a classical relation $(f, g) = k$ where k is a function of the p and q, there exists a quantummechanical relation $\boldsymbol{tg} - \boldsymbol{gf} = \boldsymbol{ihk}$.

The conditions a and e of [3,2] are the "translation" of:

$$(x_i, x_k) = 0; \quad (p_i x_k) = -\delta_{ik}; \quad (p_i, p_k) = 0$$

$$\dot{f} = (f, \mathrm{H}).$$

By translating the classical equations in rectangular coordinates for a system containing n particles we arrive at a matrix formulation which by the method of [3, 1] may be proved to be equivalent to the wave equation for n particles.

3,4. Matrix mechanics in general coordinates.

The argumentation the outline of which was given in the preceding section, does not only apply to the description of elementary particles in rectangular coordinates. If we describe a classical

system in arbitrary coordinates and take over the P . B's into quantum theory, both arguments — formal analogy and principle of correspondence — would apply as well as in the case of rectangular coordinates. It is however in general impossible in this way to construct an unambiguous analogon to the classical theory: if we meet with a term containing two factors the P . B of which does not vanish and that therefore do not commute in quantum theory, we are at a loss; we do not know whether we have to write pq or qp or perhaps $(pq + qp)/2$. But it can happen that no difficulties of this kind occur and now the problem arises:

Can the quantummechanical formulations obtained this way, also be deduced from the Schrödinger equation in rectangular coordinates?

Once more: from the classical equations in rectangular coordinates one can deduce an infinity of other formulations. To some of these formulations it will be possible unambiguously to construct a quantum mechanical analogon. Are all the quantum mechanical formulations obtained, equivalent to each other?

This question — it may be regarded as a problem in pure mathematics — does not seem quite easy to answer, especially because of the large number of possibilities; we can for example by no means confine ourselves to canonical transformations: just in the case of the rigid body the simple Eulerian treatment is based on the introduction of certain quantities (viz. the angular momenta) that cannot be regarded as new canonical variables. Therefore one cannot be quite sure that it is impossible to construct exceptional cases. But still, if we have a natural looking formulation, every phycisist will be convinced that it will give right results.

4. Matrix mechanics of the rigid body.

Our matrix theory of the rigid body will be obtained by taking over the P . B relations of [I 14]. In doing so we automatically introduce the assumption that, just as in classical mechanics, internal motion has no influence on the motion of our system as a whole. (The legitimacy of this assumption for real systems

will be discussed in the last chapter). In [2, 1] the same assumption was introduced in the wave mechanical formulation and the general problem formulated in [3, 4] takes the form: is the "matrix mechanics of the rigid body" equivalent to the "wave mechanics of the rigid body". We will be able to give a direct proof of the equivalence. If the two formulations were not equivalent we would be in a rather unpleasant position. For both formulations look quite satisfactory and as long as we do not deduce the existence of rigid bodies from the fundamental equations there is no reason to prefer one of them.

In the next sections we will discuss the matrix problem and until further notice the reader may forget everything we have said about the wave mechanical formulation.

4,1. Fundamental relations.

By translating the P . B's of [I 14] we arrive at the following relations (we will no longer distinguish matrices by fat letters).

(1) $$P_1P_2 - P_2P_1 = ihP_3$$
and so on.

(2) $$P_1K_{2i} - K_{2i}P_1 = K_{1i}P_2 - K_{1i} = ihK_{3i}$$
and so on, for all i.

(3) $$K_{ik}K_{lm} - K_{lm}K_{ik} = 0$$
for all i, k, l, m.

(4) $$Q_iP_k - P_kQ_i = 0$$
for all i, k.

(5) $$Q_1K_{i2} - K_{i2}Q_1 = K_{i1}Q_2 - Q_2K_{i1} = -ihK_{i3}$$
and so on, for all i.

(6) $$Q_1Q_2 - Q_2Q_1 = -ihQ_3.$$

Just as in the case of the classical P. B's, these relations may be deduced from (1) and (2) (that are general relations for the components of angular momentum and a vector depending on coordinates only) together with the equations:

(7) $$P_i = \sum_k K_{ik}Q_k; \quad Q_i = \sum_k K_{ki}P_k$$

and the orthogonality relations for the K_{ik}:

(8) $$\sum_l K_{il}K_{kl} = \delta_{ik},$$

(9) $$\text{Det} \parallel K_{lm} \parallel = +1.$$

The Hamiltonian is given by:

(10) $$H = \tfrac{1}{2}\left(\frac{1}{A_1}Q_1^2 + \frac{1}{A_2}Q_2^2 + \frac{1}{A_3}Q_3^2\right).$$

The equation of motion

(11) $$ih\dot{f} = fH - Hf$$

which (as in classical mechanics) must hold for any of the P_i, Q_k, K_{ik}, gives:

(12) $$\dot{P}_i = 0$$

as P_i commutes with all Q_k,

(13) $$\dot{Q}_1 = \tfrac{1}{2}(Q_2Q_3 + Q_3Q_2)\left(\frac{1}{A_3} - \frac{1}{A_2}\right)$$
and so on,

the Eulerian equations in a "symmetrized" form;

(14) $$\dot{K}_{i1} = \frac{1}{2A_2}(Q_2K_{i3} + K_{i3}Q_2) - \frac{1}{2A_3}(Q_3K_{i2} + K_{i2}Q_3)$$
and so on.

4,2. Method of solution.

We have to find a matrix representation for our quantities satisfying (apart from the equations (1)—(10) which is the meaning of the word representation) the conditions:

a. All matrices are Hermitean,

b. H is a diagonal matrix.

We do not need to take into account (11) (see [3,2]).

We will first determine a matrix representation — we call it the S-representation — on which we, instead of *b*, impose the conditions:

c. P_3 diagonal matrix,

d. Q_3 diagonal matrix.

As P_3 commutes with H it is possible to satisfy *b* and *c* at the same time. If $A_1 = A_2$ also Q_3 commutes with H. In the case of a symmetrical body the S-representation satisfies *b*. In the general case it does not satisfy *b*. To find the correct representation we have to solve algebraical equations of finite degree. The solution can however not be written down explicitly.

5. Auxiliary theorem A.
If three quantities, B_1, B_2, B_3, satisfy the relations:

(1*a*) $$B_1B_2 - B_2B_1 = iB_3,$$

(1*b*) $$B_2B_3 - B_3B_1 = iB_1,$$

(1*c*) $$B_3B_1 - B_1B_3 = iB_2,$$

then there corresponds to every $j \geqslant 0$ and half an integer, one and only one irreducible matrix representation of these quantities, with the properties:

(2) $$B_1^2 + B_2^2 + B_3^2 = j(j+1)1,$$
it is $(2j+1)$ dimensional,

the eigenvalues of any of the three quantities are: j, $(j-1)$, $\ldots$, $-j+1$, $-j$.

We choose B_3 as diagonal matrix, label rows and columns with the corresponding diagonalelement m of B_3 and introduce the notation:

(3*a*) $$B_I = B_1 + iB_2,$$

(3*b*) $$B_{II} = B_1 - iB_2;$$

then we have:

(4) $$(m \mid B_3 \mid m) = m,$$

(5) $$(m \mid B_I \mid m-1) = \sqrt{(j+m)(j-m+1)},$$

(6) $$(m \mid B_{II} \mid m+1) = \sqrt{(j-m)(j+m+1)},$$

all other matrix elements vanish.

We call these special matrices $M_i(j)$.

The most general form of our representation is given by: $SM_i(j)S^{-1}$ where S is a unitary matrix.

For a proof of this theorem compare the references given at the end of the book.

5,1. Auxiliary theorem B.
If three quantities, V_1, V_2, V_3, satisfy the relations

(1) $$B_1V_2 - V_2B_1 = B_2V_1 - V_1B_2 = iV_3$$
and so on,

where B_i is a reducible matrix (Stufenmatrix),

(2) $$(j_1, m_1 \mid B_i \mid m_2, j_2) = \delta_{j_1, j_2} \cdot (m_1 \mid M_i(j_1) \mid m_2),$$

we have (again writing $V_I = V_1 + iV_2$, $V_{II} = V_1 - iV_2$):

$$(j, m \mid V_I \mid m-1, j) = (j \mid A \mid j) \cdot \sqrt{(j+m)(j-m+1)}$$
(3) $$(j, m \mid V_{II} \mid m+1, j) = (j \mid A \mid j) \cdot \sqrt{(j-m)(j+m+1)}$$
$$(j, m \mid V_3 \mid m, j) = (j \mid A \mid j) \cdot m.$$

$$(j, m \mid V_I \mid m-1, j-1) =$$
$$= -(j \mid A \mid j-1) \cdot \sqrt{(j+m)(j+m-1)}$$
(4) $$(j, m \mid V_{II} \mid m+1, j-1) =$$
$$= (j \mid A \mid j-1) \cdot \sqrt{(j-m)(j-m-1)}$$
$$(j, m \mid V_3 \mid m, j-1) = (j \mid A \mid j-1) \cdot \sqrt{(j+m)(j-m)}.$$

$$(j, m \mid V_I \mid m-1, j+1) = (j \mid A \mid j+1) \cdot \sqrt{(j-m+1)(j-m+2)}$$
(5) $$(j, m \mid V_{II} \mid m+1, j+1) =$$
$$= -(j \mid A \mid j+1) \cdot \sqrt{(j+m+1)(j+m+2)}$$
$$(j, m \mid V_3 \mid m, j+1) = (j \mid A \mid j+1) \cdot \sqrt{(j+m+1)(j-m+1)}$$

All other matrix elements vanish. We will in the following use the abbreviation:

(6) $$(j_1, m_1 \mid V_i \mid m_2, j_2) = (j_1 \mid A \mid j_2) \cdot (m_1 \mid F_i(j_1, j_2) \mid m_2).$$

The $(j_1 \mid A \mid j_2)$ have to be Hermitean and to vanish unless $(j_1 - j_2) = 0, \pm 1$; otherwise they are arbitrary. $F_i(j_1, j_2)$ is a matrix with $(2j_1 + 1)$ rows and $(2j_2 + 1)$ columns.

If in (2) we take instead of $M_i(j_1)$, $S(j_1)M_i(j_1)S(j_1)^{-1}$ we have to take:

(7) $$S(j_1) \cdot F_i(j_1, j_2) \cdot S^{-1}(j_2)$$

instead of F_i.

If the numbers $(j_1 \mid A \mid j_2)$ do not vanish for $j_1 - j_2 = 0, \pm 1$ there are two irreducible representations for B_i, V_k. In the first one j takes the values 0, 1, 2 in the second one $j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots\ldots$

For a proof of our theorem compare the references given at the end of the book.

6. S-representation of P_i, Q_k.

It follows from [5]: the irreducible representations of P_i satisfying [4,2 *c*] are given by $hM_i(j)$, for the irreducible representations of Q_i we may take:

(1*a*, *b*, *c*). $Q_1 = hM_1(j)$, $Q_2 = -hM_2(j)$, $Q_3 = hM_3(j)$

(this amounts to taking $Q_i = \widetilde{M}_i(j) = \overline{M}_i(j)$ where $\sim$ means that we interchange rows and columns).

(1) $$\sum Q_i^2 = \sum P_i^2 = I$$

(square of total angular momentum) commutes with P_i, Q_k, H. We will choose it as a diagonalmatrix. The possible eigenvalues are $h^2 \cdot j(j+1)$. P_i, Q_k, H fall into pieces characterized by a certain value j_1 of j. In such a j_1, j_1 section the only irreducible representation of P_i that can occur is $hM_i(j_1)$, the only irreducible representation of Q_i $h\overline{M}_i(j)$. But these representations may occur several times. As all P_i commute with all Q_k and only a matrix proportional unity commutes with all matrices of an irreducible set, it follows (if we call the eigenvalues of Q_3 *hs*, of P_3 *hm*):

(3) $$(j_1, m_1, s_1 \mid Q_i \mid s_2, m_2, j_1) = h \cdot \delta_{m_1 m_2} \cdot (s_1 \mid M_i(j_1) \mid s_2),$$

(4) $$(j_1, m_1, s_1 \mid P_i \mid s_2, m_2, j_1) = h \cdot \delta_{s_1 s_2} \cdot (m_1 \mid M_i(j_1) \mid m_2),$$

One such j_1, j_1 section can occur only once, for there are no other quantities commuting with P_3, Q_3, I, the eigenvalues of which could be used to distinguish two different j, j sections.

6,1. S-representation of *H*.

As H depends on the Q_i only, we find at once:

(1) $$(j_1, m_1, s_1 \mid H \mid s_2, m_2, j_2) = \delta_{j_1, j_2} \cdot \delta_{m_1, m_2} \cdot (s_1 \mid H(j_1) \mid s_2).$$

For $(s_1 \mid H(j) \mid s_2)$ we find:

a. Case of a symmetrical body ($A_1 = A_2$).

(2) $$H = \tfrac{1}{2}\left[\frac{1}{A_1}(Q_1^2 + Q_2^2) + \frac{1}{A_3}Q_3^2\right] =$$

$$= \tfrac{1}{2}\left[\frac{1}{A_1}(Q_1^2 + Q_2^2 + Q_3^2) + \left(\frac{1}{A_3} - \frac{1}{A_1}\right)Q_3^2\right],$$

(3) $$(s_1 \mid H(j) \mid s_2) = \delta_{s_1 s_2} \cdot \frac{h^2}{2}\left[\frac{1}{A_1} \cdot j(j+1) + \left(\frac{1}{A_3} - \frac{1}{A_1}\right)s_1^2\right].$$

H is a diagonal matrix, as was to be expected.

b. Case of an assymmetric body.

$$(s-2 \mid H \mid s) = (s \mid H \mid s-2) =$$

(4) $$= h^2\left(\frac{1}{8A_1} - \frac{1}{8A_2}\right)\sqrt{(j+s)(j+s-1)(j-s+1)(j-s+2)}.$$

(5) $$(s \mid H \mid s) = h^2\left[\left(\frac{1}{4A_1} + \frac{1}{4A_2}\right)\{j(j+1) - s^2\} + \frac{1}{2A_3} \cdot s^2\right].$$

In order to make H a diagonal matrix we must take instead of $Q_i = h\overline{M}_i(j)$ $Q_i = hS(j)\overline{M}_i(j)S^{-1}(j)$ and choose S such that SHS^{-1} is a diagonalmatrix. The eigenvalues are the roots of:

(6) $$\text{Det} \parallel (s_1 \mid H \mid s_2) - E\delta_{s_1 s_2} \parallel = 0,$$

and the matrixelements of S, $(E \mid S \mid s)$, satisfy the equations:

(7) $$\sum_{s', s''} (E_1 \mid S \mid s')(s' \mid H \mid s'')(s'' \mid S \mid E_2) = E_1 \delta_{E_1 E_2}$$

where

(8) $$\sum_{s'} (E_1 \mid S \mid s')(s' \mid S \mid E_2) = \delta_{E_1 E_2},$$

(9) $$(s \mid S \mid E) = \overline{(E \mid S \mid s)},$$

and accordingly:

(10) $\sum_{s''} (s' \mid \mathrm{H} \mid s'')\,(s'' \mid \mathrm{S} \mid \mathrm{E}_1) = \mathrm{E}_1 \,.\, (s' \mid \mathrm{S} \mid \mathrm{E}_1).$

6,2. S-representation of the K_{lm}.

By applying [5,1] to the equations [4,1 (2)] we get:

(1) $$(j_1,\ m_1,\ s_1 \mid \mathrm{K}_{ik} \mid s_2,\ m_2,\ j_2) = \\ = (j_1,\ s_1 \mid \mathrm{K}_k \mid s_2,\ j_2) \,.\, (m_1 \mid \mathrm{F}_i(j_1,\ j_2) \mid m_2)$$

(K_k arbitrary for $j_1 - j_2 = 0, \pm 1$, otherwise zero) and from [4,1 (5)] we infer (observe that we again must take $\widetilde{\mathrm{F}_i} = \overline{\mathrm{F}_i}$ in stead of F_i):

(2) $$(j_1,\ m_1,\ s_1 \mid \mathrm{K}_{ik} \mid s_2,\ m_2,\ j_2) = \\ = (j_1,\ m_1 \mid \mathrm{L}_i \mid m_2,\ j_2) \,.\, \overline{(s_1 \mid \mathrm{F}_k(j_1,\ j_2) \mid s_2)}.$$

Combination of (1) and (2) gives:

(3) $$(j_1,\ m_1,\ s_1 \mid \mathrm{K}_{ik} \mid s_2,\ m_2,\ j_2) = \\ = (j_1 \mid \mathrm{A} \mid j_2) \,.\, (m_1 \mid \mathrm{F}_i(j_1,\ j_2) \mid m_2) \,.\, \overline{(s_1 \mid \mathrm{F}_k(j_1,\ j_2) \mid s_2)}$$

where $(j_1 \mid \mathrm{A} \mid j_2)$ is arbitrary for $j_1 - j_2 = 0, \pm 1$, otherwise zero. To determine $(j \mid \mathrm{A} \mid j)$ we use [4,1 (7)] in the form:

(4) $$\mathrm{P}_i = \tfrac{1}{2}\mathrm{K}_{i\mathrm{I}}\mathrm{Q}_{\mathrm{II}} + \tfrac{1}{2}\mathrm{K}_{i\mathrm{II}}\mathrm{Q}_{\mathrm{I}} + \mathrm{K}_{i3}\mathrm{Q}_3;$$

applying (3) and [6 (3)] we find, multiplying the matrices and adding:

(5) $$(j_1,\ m_1,\ s_1 \mid \mathrm{P}_i \mid s_2,\ m_2,\ j_2) = \\ = h \,.\, \delta_{j_1 j_2} \,.\, \delta_{s_1 s_2} \,.\, j_1(j_1+1) \,.\, (j_1 \mid \mathrm{A} \mid j_1)\,(m_1 \mid \mathrm{M}_i(j) \mid m_2)$$

and accordingly:

(6) $$(j \mid \mathrm{A} \mid j) = \frac{1}{j(j+1)}.$$

To find $(j \mid \mathrm{A} \mid j+1)$ and $(j \mid \mathrm{A} \mid j-1)$ we use the condition that all K_{ik} must commute with each other. The equation:

(7) $$\mathrm{K}_{\mathrm{I}\,\mathrm{II}}\mathrm{K}_{\mathrm{II}\,\mathrm{I}} - \mathrm{K}_{\mathrm{II}\,\mathrm{I}}\mathrm{K}_{\mathrm{I}\,\mathrm{I}} = 0$$

gives for the j, j elements (remark that $(j \mid \mathrm{A} \mid j-1) = \overline{(j-1 \mid A \mid j)}$)

(8) $$(j \mid \mathrm{A} \mid j)^2 - (2j-1)\,|(j \mid \mathrm{A} \mid j-1)|^2 + (2j+3)\,|(j \mid \mathrm{A} \mid j+1)|^2 = 0.$$

$$\mathrm{K}_{\mathrm{I}\,\mathrm{II}}\mathrm{K}_{\mathrm{II}\,\mathrm{II}} - \mathrm{K}_{\mathrm{II}\,\mathrm{II}}\mathrm{K}_{\mathrm{I}\,\mathrm{I}} = 0$$

leads to:

(10) $$j(j+1)\,(j \mid \mathrm{A} \mid j)^2 + j(j-1)\,(2j-1)\,|(j \mid \mathrm{A} \mid j-1)|^2 - \\ - (j+1)\,(j+2)\,(2j+3)\,|(j \mid \mathrm{A} \mid j+1)|^2 = 0.$$

(8), (10), and (6) give:

(11) $$(j \mid \mathrm{A} \mid j-1) = \frac{1}{j\sqrt{(2j-1)\,(2j+1)}};$$

(12) $$(j \mid \mathrm{A} \mid j+1) = \frac{1}{(j+1)\sqrt{(2j+1)\,(2j+3)}};$$

apart from a phase factor that is of no interest, since it can be removed by transformation with a diagonal matrix.

There is no difficulty in verifying that all conditions are satisfied.

6,3. The K_{lm} for an assymmetric body.

It is evident which change has to be made in the case of an assymmetric body: in [6,2 (3)] we have to take instead of

$$\overline{(s_1 \mid \mathrm{F}_i(j_1, j_2 \mid s_2)}:$$

$$(\mathrm{E}_1 \mid \mathrm{F}_i(j_1, j_2) \mid \mathrm{E}_2) = \sum_{s',\,s''} (\mathrm{E}_1 \mid \mathrm{S} \mid s')\ \overline{(s' \mid \mathrm{F}_i(j_1, j_2) \mid s'')}\ (s'' \mid \mathrm{S} \mid \mathrm{E}_2)$$

where $(\mathrm{E}_1 \mid \mathrm{S} \mid s')$ are the quantities defined in [6,1].

6,4. Two solutions.

We have (compare [5,1]) obtained two irreducible solutions. For the first one $j = 0,\ 1,\ 2 \ldots$. for the second one $j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2} \ldots$.

7. Transition probabilities.

The matrix elements of the K_{lm} determine the transition probabilities of our system. For these probalities are given by the square modul of the matrix elements of the electric moment. Now the components of the electric moment in the moving system, $\varepsilon_1,\ \varepsilon_2,\ \varepsilon_3$, depend on the internal motion only and we may therefore treat them as ordinary numbers (that are, strictly

speaking, the matrix elements of ε_i with respect to the internal motion). The components in the ***f***-system are given by:

$$\delta_i = \sum_l K_{il}\varepsilon_l. \tag{1}$$

This formula applies as well to the case that ε_l is the matrix element corresponding to a transition of the internal motion from one state to another as to the case that the internal motion stays the same.

If our system is put into a very weak magnetic or electric field having the direction of the z-axis, our matrix representation will, to a first approximation, not be changed, but the states with different m will have a slightly different energy and it is possible to distinguish between transitions for which the final and initial state only differ with respect to m. If however no such field is present, only the sum of the probabilities belonging to the different possible values of m has a meaning. We have to calculate:

$$\begin{aligned} |\, d_i \,|^2 &= \sum_{m_1=-j_1}^{m_1=j_1} \sum_{m_2=-j_2}^{m_2=j_2} |\, \sum_k (j_1, m_1, \mathrm{E}_1 \mid \mathrm{K}_{ik} \mid \mathrm{E}_2, m_2, j_2)\varepsilon_k \,|^2 = \\ &= \left\{ \sum_{m_1=-j_1}^{m_1=j_1} \sum_{m_2=-j_2}^{m_2=j_2} |\, (j_1 \mid \mathrm{A} \mid j_2)(m_1 \mid \mathrm{F}_i(j_1, j_2) \mid m_2) \,|^2 \right\} \cdot \\ &\cdot |\, (\mathrm{E}_1 \mid \sum_k \mathrm{F}_k(j_1, j_2) \cdot \varepsilon_k \mid \mathrm{E}_2) \,|^2 = \\ &= (j_1 \mid \mathrm{C}_i \mid j_2) \cdot |\, (\mathrm{E}_1 \mid \sum_k \mathrm{F}_k(j_1, j_2) \cdot \varepsilon_k \mid \mathrm{E}_2) \,|^2 \end{aligned} \tag{2}$$

say. The result of the summation does not depend on the index i: the intensity of the light emitted is the same for any direction of the electric vector. We are mainly interested in the total transition probability, which is determined by:

$$\sum_i |\, d_i \,|^2 = (j_1 \mid \mathrm{C} \mid j_2) \cdot |\, (\mathrm{E}_1 \mid \sum_k \mathrm{F}_k(j_1, j_2)\varepsilon_k \mid \mathrm{E}_2) \,|^2. \tag{3}$$

where

$$(j_1 \mid \mathrm{C} \mid j_2) = 3(j_1 \mid \mathrm{C}_i \mid j_2). \tag{4}$$

We find:

$$(j \mid \mathrm{C} \mid j) = \frac{2j+1}{j(j+1)}, \tag{5}$$

$$(j \mid \mathrm{C} \mid j-1) = \frac{1}{j}, \tag{6}$$

$$(j \mid \mathrm{C} \mid j+1) = \frac{1}{j+1}. \tag{7}$$

For a symmetrical body we use (3) in the form:

$$\sum_i |\, d_i \,|^2 = (j_1 \mid \mathrm{C} \mid j_2) \cdot |\, (s_1 \mid \tfrac{1}{2}\mathrm{F}_\mathrm{I}\varepsilon_\mathrm{I} + \tfrac{1}{2}\mathrm{F}_\mathrm{II}\varepsilon_\mathrm{II} + \mathrm{F}_3\varepsilon_3 \mid s_2) \,|^2. \tag{8}$$

Using [6,2 (3) (6) (11) (12)] we find for $\sum_i |\, d_i \,|^2$:

$$j \to j,\quad s \to s-1 \qquad \tfrac{1}{4} \cdot \frac{2j+1}{j(j+1)} \cdot (j+s)(j-s+1) \cdot (|\, \varepsilon_1 \,|^2 + |\, \varepsilon_2 \,|^2), \tag{9}$$

$$j \to j,\quad s \to s+1 \qquad \tfrac{1}{4} \cdot \frac{2j+1}{j(j+1)} \cdot (j-s)(j+s+1) \cdot (|\, \varepsilon_1 \,|^2 + |\, \varepsilon_2 \,|^2), \tag{10}$$

$$j \to j,\quad s \to s \qquad \frac{2j+1}{j(j+1)} \cdot s^2 \cdot |\, \varepsilon_3 \,|^2. \tag{11}$$

$$j \to j-1,\quad s \to s-1 \qquad \tfrac{1}{4} \cdot \frac{1}{j} \cdot (j+s)(j+s-1) \cdot (|\, \varepsilon_1 \,|^2 + |\, \varepsilon_2 \,|^2), \tag{12}$$

$$j \to j-1,\quad s \to s+1 \qquad \tfrac{1}{4} \cdot \frac{1}{j} \cdot (j-s)(j-s-1) \cdot (|\, \varepsilon_1 \,|^2 + |\, \varepsilon_2 \,|^2), \tag{13}$$

$$j \to j-1,\quad s \to s \qquad \frac{1}{j} \cdot (j+s)(j-s) \cdot |\, \varepsilon_3 \,|^2. \tag{14}$$

$$j \to j+1,\quad s \to s-1 \qquad \tfrac{1}{4} \cdot \frac{1}{j+1} \cdot (j-s+1)(j-s+2) \cdot (|\varepsilon_1|^2 + |\varepsilon_2|^2), \tag{15}$$

$$j \to j+1,\quad s \to s+1 \qquad \tfrac{1}{4} \cdot \frac{1}{j+1} \cdot (j+s+1)(j+s+2) \cdot (|\, \varepsilon_1 \,|^2 + |\varepsilon_2|^2), \tag{16}$$

$$j \to j+1,\quad s \to s \qquad \frac{1}{j+1} \cdot (j+s+1)(j-s+1) \cdot |\, \varepsilon_3 \,|^2. \tag{17}$$

To obtain the total energy emitted per unit time we have to multiply these expressions by:

$$\tfrac{4}{3}\frac{(2\pi\nu)^4}{c^3},$$

where ν is the frequency emitted (see [3 (7)]).

8. Construction of a wave equation.

The algebraical problem is solved. Before giving a nearer discussion of the energy levels and intensities in the case of an assymmetric body, we will further develop the general theory. We will show how it is possible, starting from the algebraical formulation, to construct a wave equation. This wave equation will turn out to be identical with that of [2, 2 (4)]; the equivalence of matrix mechanics and wave mechanics of the rigid body (see [4]) is then proved.

Let us assume that there exists a wave equation giving results identical with those of matrix calculus. To a state of our system will correspond a function $f(\vartheta^\lambda, \alpha)$, where ϑ^λ are the Eulerian angles and α represents the three quantum numbers (j, m, s in the case of a symmetric body). The K_{ik} will be given by the ordinary expressions for the cosines between ***f***- and ***k***-system as functions of the Eulerian angles [I 4 (7)] and instead of the P_i and Q_k there will come certain operators; we call these operators $\mathcal{P}_i$ and $\mathcal{Q}_k$ resp. and write $K_{ik}(\vartheta^\lambda) = \mathcal{K}_{ik}$. The matrix representation is now obtained by calculating

$$(\alpha \mid P_i \mid \beta) = \int \overline{f(\vartheta^\lambda, \alpha)}\,\mathcal{P}_i f(\vartheta^\lambda, \alpha).$$

$$\mathcal{P}_i f(\vartheta^\lambda, \alpha) = \sum_\beta (\beta \mid P_i \mid \alpha)\, f(\vartheta^\lambda, \beta).$$

The relations of [4, 1] must also hold for the $\mathcal{P}_i$, $\mathcal{Q}_k$, $\mathcal{K}_{ik}$.

For instance:

(1) $$(\mathcal{P}_1\mathcal{K}_{2i} - \mathcal{K}_{2i}\mathcal{P}_1)\psi = ih\mathcal{K}_{3i}\psi,$$

for arbitrary ψ. This condition is satisfied if $\mathcal{P}_1$ is a differential operator of the first order:

(2) $$\mathcal{P}_1 = \pi_1{}^\lambda \frac{\partial}{\partial\vartheta^\lambda}$$

and

(3) $$\pi_1{}^\lambda \frac{\partial}{\partial\vartheta^\lambda}\mathcal{K}_{2i}(\vartheta^\lambda) = ih\mathcal{K}_{3i}.$$

In [I 13] we had deduced the classical relation:

(4) $$(P_1,\ K_{2i}) = K_{3i}.$$

As $P_1 = p_1{}^\lambda \pi_\lambda$ this becomes:

(5) $$-\,p_1{}^\lambda \frac{\partial}{\partial\vartheta^\lambda}K_{2i} = K_{3i}.$$

We are thus led to the assumption:

(6) $$\mathcal{P}_1 = -\,ihp_1{}^\lambda \frac{\partial}{\partial\vartheta^\lambda}$$

and by the same reasoning:

(7) $$\mathcal{P}_i = -\,ihp_i{}^\lambda \frac{\partial}{\partial\vartheta^\lambda},$$

(8) $$\mathcal{Q}_i = -\,ihq_i{}^\lambda \frac{\partial}{\partial\vartheta^\lambda}.$$

These operators have a simple geometrical meaning:

(9) $$-\frac{i}{h}\varepsilon\mathcal{P}_i f(\vartheta^\nu) \quad \text{resp.} \quad -\frac{i}{h}\varepsilon\mathcal{Q}_i f(\vartheta^\nu)$$

is the change of the function f when an infinitesimal rotation ε about $\boldsymbol{f}_i$ resp. $\boldsymbol{k}_i$ is carried out. If the rotation changes ϑ^ν into $\vartheta^{*\nu}$ the transformed function f^* is defined by the equation $f^*(\vartheta^{*\nu}) = f(\vartheta)$. The change is given by:

(10) $$f^*(\vartheta^*) - f(\vartheta^*) = f(\vartheta^\nu) - f(\vartheta^*) =$$

$$= -\,\varepsilon\frac{\vartheta^{*\lambda} - \vartheta^\lambda}{\varepsilon}\frac{\partial}{\partial\vartheta^\lambda}f(\vartheta^\nu).$$

But we have:

$$\lim_{\varepsilon \to 0} \frac{\vartheta^{*\lambda} - \vartheta^{\lambda}}{\varepsilon} = p_i^{\lambda} \quad \text{resp.} \quad q_i^{\lambda}$$

(see [I 6,2]).

In order to verify that $\mathcal{P}_i$, $\mathcal{Q}_k$ also satisfy [4,1 (1) (4) (6)] we have only to use the relations:

(11) $$p_1{}^{\lambda} \frac{\partial}{\partial \vartheta^{\lambda}} p_2{}^{\mu} - p_2{}^{\lambda} \frac{\partial}{\partial \vartheta^{\lambda}} p_1{}^{\mu} = - p_3{}^{\mu}$$

and so on,

(12) $$p_i^{\lambda} \frac{\partial}{\partial \vartheta^{\lambda}} q_k^{\mu} - q_k^{\lambda} \frac{\partial}{\partial \vartheta^{\lambda}} p_i^{\mu} = 0$$

all i, k,

(13) $$q_1{}^{\lambda} \frac{\partial}{\partial \vartheta^{\lambda}} q_2{}^{\mu} - q_2{}^{\lambda} \frac{\partial}{\partial \vartheta^{\lambda}} q_1{}^{\mu} = + q_3{}^{\mu}$$

and so on,

that were also used in calculating the classical P . B's.

Herewith we have proved: the algebraical treatment is equivalent to a wave mechanical treatment with the wave equation

(14) $$\left[- \frac{h^2}{2} \sum_i \frac{1}{A_i} \left\{ q_i^{\lambda} \frac{\partial}{\partial \vartheta^{\lambda}} q_i^{\mu} \frac{\partial}{\partial \vartheta^{\mu}} \right\} \right] \psi = E\psi.$$

In [2,2 (4)] we had obtained the equation

(15) $$\left[- \frac{h^2}{2} \sum_i \frac{1}{A_i} \left\{ \frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta^{\lambda}} \sin \vartheta \, . \, q_i^{\lambda} q_i^{\mu} \frac{\partial}{\partial \vartheta^{\mu}} \right\} \right] \psi = E\psi.$$

To prove the identity of these two equations one has to verify:

(16) $$\frac{\partial}{\partial \vartheta^{\lambda}} (\sin \vartheta \, . \, q_i^{\lambda}) = 0$$

which is easily done by using the expressions for q_i^{λ} given in [I 6,2].

The explicit expressions for $\mathcal{P}_i$ and $\mathcal{Q}_k$ are:

(17a) $$\mathcal{P}_1 = - ih \left[\cos \psi \, . \, \frac{\partial}{\partial \vartheta} - \frac{\cos \vartheta \sin \psi}{\sin \vartheta} \, . \, \frac{\partial}{\partial \psi} + \frac{\sin \psi}{\sin \vartheta} \, . \, \frac{\partial}{\partial \varphi} \right].$$

(17b) $$\mathcal{P}_2 = - ih \left[\sin \psi \, . \, \frac{\partial}{\partial \vartheta} + \frac{\cos \vartheta \cos \psi}{\sin \vartheta} \, . \, \frac{\partial}{\partial \psi} - \frac{\cos \psi}{\sin \vartheta} \, . \, \frac{\partial}{\partial \varphi} \right].$$

(17c) $$\mathcal{P}_3 = - ih \, . \, \frac{\partial}{\partial \psi}.$$

(18a) $$\mathcal{Q}_1 = - ih \left[\cos \varphi \, . \, \frac{\partial}{\partial \vartheta} + \frac{\sin \varphi}{\sin \vartheta} \, . \, \frac{\partial}{\partial \psi} - \frac{\cos \vartheta \sin \varphi}{\sin \vartheta} \, . \, \frac{\partial}{\partial \varphi} \right].$$

(18b) $$\mathcal{Q}_2 = - ih \left[- \sin \varphi \, . \, \frac{\partial}{\partial \vartheta} + \frac{\cos \varphi}{\sin \vartheta} \, . \, \frac{\partial}{\partial \psi} - \frac{\cos \vartheta \cos \varphi}{\sin \vartheta} \, . \, \frac{\partial}{\partial \varphi} \right].$$

(18c) $$\mathcal{Q}_3 = - ih \, . \, \frac{\partial}{\partial \varphi}.$$

9. Wave equation and wave functions for a symmetrical body. In the case of a symmetrical body the wave equation becomes:

(1) $$- \frac{h^2}{2} \left[\frac{1}{A_1} \left(\frac{\partial^2}{\partial \vartheta^2} + \frac{\cos \vartheta}{\sin \vartheta} \, . \, \frac{\partial}{\partial \vartheta} + \frac{1}{\sin^2 \vartheta} \, . \, \frac{\partial^2}{\partial \psi^2} - \frac{2 \cos \vartheta}{\sin^2 \vartheta} \, . \, \frac{\partial}{\partial \varphi} \, . \, \frac{\partial}{\partial \psi} + \right. \right.$$
$$\left. \left. + \frac{\cos^2 \vartheta}{\sin^2 \vartheta} \, . \, \frac{\partial^2}{\partial \varphi^2} \right) + \frac{1}{A_3} \, . \, \frac{\partial^2}{\partial \varphi^2} \right] u = Eu.$$

In the matrix treatment we found that we could choose P_3 and Q_3 as diagonalmatrices, the eigenvalues being hm resp. hs; that means:

(2) $$\mathcal{P}_3 u = hmu,$$

(3) $$\mathcal{Q}_3 u = hsu,$$

(4) $$u = e^{i(m\psi + s\varphi)} f_{ms}(\vartheta).$$

If we want the eigenfunctions to be one-valued we must confine ourselves to the solution $j = 0, 1, 2, 3 \ldots$.

If we drop this condition we must expect to find a set of two-valued eigenfunctions, forming together with the one-valued

functions a complete orthogonal set for all two-valued functions. To this question, that is important in connection with the electronic spin, we will return later on. For the present we will confine ourselves to the case j integer.

For f_{ms} we find the equation:

$$(5)\quad \left(\frac{\partial^2}{\partial\vartheta^2}+\frac{\cos\vartheta}{\sin\vartheta}\cdot\frac{\partial}{\partial\vartheta}-\frac{m^2}{\sin^2\vartheta}+2ms\frac{\cos\vartheta}{\sin^2\vartheta}-\frac{s^2}{\sin^2\vartheta}\right)f_{ms}+\lambda f_{ms}=0,$$

where

$$(6)\quad \lambda=\mathrm{A}_1\left(\frac{2\mathrm{E}}{h^2}-\frac{s^2}{\mathrm{A}_3}\right)+s^2.$$

The possible values of λ are, as follows from the matrix theory, $j(j+1)$. Substituting $z=\cos\vartheta$ we get:

$$(7)\quad \left[(1-z^2)\frac{d^2}{dz^2}-2z\frac{d}{dz}-\frac{s^2-2smz+m^2}{1-z^2}\right]f+\lambda f=0.$$

For $m=0$ this equation is reduced to the equation for the associated Legendre polynomials and we have:

$$(8)\quad u(\vartheta^\lambda;\ m=0,\ s,\ j)=e^{is\varphi}\,e^{i\alpha(s,j)}\,\mathrm{N}(s,j)\,\mathrm{P}_j^{|s|}(\cos\vartheta),$$

where

$$(9)\quad \mathrm{P}_j^{|s|}(z)=(1-z^2)^{\frac{|s|}{2}}\cdot\frac{d^{j+|s|}}{dz^{j+|s|}}(1-z^2)^j$$

and $\mathrm{N}(s,j)$ a positive real normalization factor. We will determine in which way the phase constants $\alpha(s,j)$ must be chosen in order to obtain for $\mathrm{Q_I}$, $\mathrm{Q_{II}}$ just the form $\mathrm{M}(j)\,.\,\mathrm{Q}_3$ has this form in any case, and that determines the representation for $\mathrm{Q_I}$ and $\mathrm{Q_{II}}$ apart from a phase factor. We have to choose $\alpha(s,j)$ such that:

$$(10)\quad (s|\mathrm{Q_I}|s+1)=2\pi\,.\,\mathrm{N}(s,j)\mathrm{N}(s+1,j)\,.\int_0^{2\pi}\!\!\int_0^{\pi} e^{-is\varphi}\,e^{-i\alpha(s,j)}\mathrm{P}_j^{|s|}(\cos\vartheta)\,.$$

$$.\left[-ihe^{-i\varphi}\left\{\frac{\partial}{\partial\vartheta}-i\frac{\cos\vartheta}{\sin\vartheta}\cdot\frac{\partial}{\partial\varphi}\right\}\right]e^{i(s+1)\varphi}\,e^{i\alpha(s+1,j)}\,.$$

$$.\,\mathrm{P}_j^{|s+1|}(\cos\vartheta)\,.\,\sin\vartheta\,d\vartheta\,.\,d\varphi$$

is real and positive. It follows:

$$(11)\quad e^{i(\alpha(s+1,j)-\alpha(s,j))}\,.\,(-ih)\int_{-1}^{1}\mathrm{P}_j^{|s|}(z)\left[-\sqrt{1-z^2}\,.\,\frac{d}{dz}+\right.$$

$$\left.+\frac{(s+1)z}{\sqrt{1-z^2}}\right]\mathrm{P}_j^{|s+1|}(z)dz$$

must be real and positive.

For $s\gtrless 0$ we have:

$$-\int_{-1}^{1}\mathrm{P}_j^{s}(z)\,(1-z^2)^{\frac{1}{2}}\frac{d}{dz}(\mathrm{P}_j^{s+1}(z))\,dz=$$

$$(12)\quad =\int_{-1}^{1}\mathrm{P}_j^{s+1}(z)\,.\,\frac{d}{dz}\left[(1-z^2)^{\frac{s+1}{2}}\,.\,\frac{d^s}{dz^s}\left\{\mathrm{P}_j(z)\right\}\right]dz=$$

$$=\int_{-1}^{1}[\,\mathrm{P}_j^{s+1}(z)]^2\,dz-\int_{-1}^{1}\frac{(s+1)z}{\sqrt{1-z^2}}\,.\,\mathrm{P}_j^{s}(z)\,\mathrm{P}_j^{s+1}(z)\,dz.$$

In order to make $(s\mid \mathrm{Q_I}\mid s+1)$ real and positive we have to make

$$e^{i(\alpha(s+1,j)-\alpha(s,j))}\,.\,(-i)$$

real and positive, that will say:

$$(13)\quad \alpha(s,j)=+\,s\,\frac{\pi}{2}+b_j.$$

For $s<0$ we have, calling $|\,s\,|=n$.

$$(14)\quad (s\mid \mathrm{Q_I}\mid s+1)=\mathrm{N}(s,j)\mathrm{N}(s+1,j)\,.\,4\pi^2\,.\,e^{i(\alpha(s+1,j)-\alpha(s,j))}\,.\,(-ih)\,.$$

$$.\int_{-1}^{1}\mathrm{P}_j^{n}(z)\left[-\sqrt{1-z^2}\,.\,\frac{d}{dz}-\frac{(n-1)z}{\sqrt{1-z^2}}\right]\mathrm{P}_j^{n-1}\,.\,dz.$$

For the integral we find:

$$-\int_{-1}^{1}[\mathrm{P}_j^{n}(z)]^2\,dz$$

and accordingly

$$e^{i(\alpha(s+1,j)-\alpha(s,j))} \cdot (+i)$$

has to be real and positive.
Thus we arrive at the general formula:

(15) $$\alpha(s, j) = |\, s \,| \cdot \frac{\pi}{2} + b_j.$$

Introducing the notation $\varphi + \frac{\pi}{2} = \chi$ (χ, ϑ are then the polar coordinates of $\boldsymbol{f}_z$ in the $\boldsymbol{k}$-system) we have:

(16) $$u(\vartheta^\lambda;\ m = 0, s, j) = e^{is\chi} \mathrm{P}_j^s(\cos\vartheta)\, \mathrm{N}(s, j)\, e^{ibj} \qquad \text{for } s \geqslant 0,$$

(17) $$u(\vartheta^\lambda;\ m = 0, s, j) = (-)^{|s|} e^{is\chi} \mathrm{P}_j^{|s|}(\cos\vartheta) \mathrm{N}(s, j) e^{ibj} \qquad \text{for } s < 0.$$

10. Nearer discussion of the assymetric body. The four classes. If we represent all our operators in the orthogonal system formed by the eigenfunctions of the symmetrical body, we will get the "S-representation". For example.

(1) $$(j_1, m_1, s_1 \mid \mathrm{H} \mid s_2, m_2, j_2) = \int \overline{u(\vartheta^\lambda;\ j_1, m_1, s_1)} \left(\frac{1}{2} \sum_i \frac{1}{\mathrm{A}_i} \mathcal{Q}_i^2\right) \cdot u(\vartheta^\lambda;\ j_2, m_2, s_2).$$

If we want to make H a diagonal matrix we have instead of $u(\vartheta^\lambda;\ j, m, s)$ to take certain linear combinations. As H is already a diagonal matrix with respect to j and m we have only to combine functions with the same j and m but different s:

(2) $$u(\vartheta^\lambda;\ j, m, \mathrm{E}) = \sum_s (s \mid \mathrm{S}(j) \mid \mathrm{E})\, u(\vartheta^\lambda;\ j, m, s).$$

The $(s \mid \mathrm{S}(j) \mid \mathrm{E})$ or abbreviated $(s \mid \mathrm{E})$ have to satisfy the equations:

(3) $$(s \mid \mathrm{H} \mid s-2)(s-2 \mid \mathrm{E}) + (s \mid \mathrm{H} \mid s)(s \mid \mathrm{E}) + (s \mid \mathrm{H} \mid s+2)(s+2 \mid \mathrm{E}) = \mathrm{E} \cdot (s \mid \mathrm{E}).$$

These equations do not connect functions for which s is even with functions for which s is odd.

The states of an assymmetric body may be divided into two

classes $\boldsymbol{O}$ and $\boldsymbol{E}$. The eigenfunctions of the $\boldsymbol{E}$-class are combinations of functions for which s is even, those of the $\boldsymbol{O}$-class combinations of functions for which s is odd.

But we may still further reduce our problem. We remark that:

(4) $$(s \mid \mathrm{H} \mid s-2) = (-s \mid \mathrm{H} \mid -s+2),$$

(5) $$(s \mid \mathrm{H} \mid s) = (-s \mid \mathrm{H} \mid -s).$$

We have:

(6) $$(s \mid \mathrm{H} \mid s+2)(s+2 \mid \mathrm{E}) + (s \mid \mathrm{H} \mid s)(s \mid \mathrm{E}) + (s \mid \mathrm{H} \mid s-2)(s-2 \mid \mathrm{E}) = \mathrm{E} \cdot (s \mid \mathrm{E}).$$

(7) $$(s \mid \mathrm{H} \mid s+2)(-s-2 \mid \mathrm{E}) + (s \mid \mathrm{H} \mid s)(-s \mid \mathrm{E}) + (s \mid \mathrm{H} \mid s-2)(-s+2 \mid \mathrm{E}) = \mathrm{E} \cdot (-s \mid \mathrm{E}).$$

If we add and subtract these equations our system is splitted up into two sets. The first one only contains the $(s \mid E) + (-s \mid E)$, the other one only the $(s \mid E) - (-s \mid E)$.

The states of an assymmetrical body may be divided into *four classes:*

$$\boldsymbol{\Theta+}, \quad \boldsymbol{\Theta-}, \quad \boldsymbol{E+}, \quad \boldsymbol{E-}.$$

For $m = 0$ we find for the wave functions, using [9 (16) (17)]:

$\boldsymbol{E+}$ functions are combinations of $\mathrm{P}_j^0(\cos\vartheta)$, $\cos 2\chi \cdot \mathrm{P}_j^2$,

$\boldsymbol{E-}$ functions are combinations of $\sin 2\chi \cdot \mathrm{P}_j^2$, ...

$\boldsymbol{O+}$ functions are combinations of $\sin\chi \cdot \mathrm{P}_j^1$, $\sin 3\chi \cdot \mathrm{P}_j^3$,

$\boldsymbol{O-}$ functions are combinations of $\cos\chi \cdot \mathrm{P}_j^1$, $\cos 3\chi \cdot \mathrm{P}_j^3$.

If we introduce the normalized quantities

$$\frac{1}{\sqrt{2}}\left[(s \mid \mathrm{E}) \pm (-s \mid \mathrm{E})\right]$$

we find for the Hamiltonians belonging to each class:

$E+$:

$$(8)\quad \begin{vmatrix} \left(\frac{h^2}{4A_1}+\frac{h^2}{4A_2}\right)\cdot j(j+1) & \sqrt{2}\left(\frac{h^2}{8A_1}-\frac{h^2}{8A_2}\right)\sqrt{j(j-1)(j+1)(j+2)} & 0 \\ \sqrt{2}\left(\frac{h^2}{8A_1}-\frac{h^2}{8A_2}\right)\sqrt{j(j-1)(j+1)(j+2)} & \left(\frac{h^2}{4A_1}+\frac{h^2}{4A_2}\right)(j(j+1)-2^2)+\frac{2^2h^2}{2A_3} & \left(\frac{h^2}{8A_1}-\frac{h^2}{8A_2}\right)\sqrt{(j+4)(j+3)(j-3)(j-2)} \\ 0 & \left(\frac{h^2}{8A_1}-\frac{h^2}{8A_2}\right)\sqrt{(j+4)(j+3)(j-3)(j-2)} & \end{vmatrix}$$

and so on.

$E-$ is obtained by omitting the first row and column.

$O\pm$:

$$(9)\quad \begin{vmatrix} \left(\frac{h^2}{4A_1}+\frac{h^2}{4A_2}\right)(j(j+1)-1)+\frac{h^2}{2A_3}\pm\left(\frac{h^2}{8A_1}-\frac{h^2}{8A_2}\right)\sqrt{(j+1)j\cdot j(j-1)} & \left(\frac{h^2}{8A_1}-\frac{h^2}{8A_2}\right)\sqrt{(j+3)(j+2)(j-2)(j-1)} \\ \left(\frac{h^2}{8A_1}-\frac{h^2}{8A_2}\right)\sqrt{(j+3)(j+2)(j-2)(j-1)} & \left(\frac{h^2}{4A_1}+\frac{h^2}{4A_2}\right)(j(j+1)-3^2)+\frac{3^2h^2}{2A_3} \end{vmatrix}$$

and so on.

10, 1. The four classes and rotations of the k-system. In our treatment Q_3 was chosen as a diagonal matrix. We may as well choose Q_1 or Q_2 as diagonalmatrix. We arrive then at another H-matrix in which the moments of inertia A_3 and A_1 resp. A_2 are interchanged. The question arises: in which way are the four classes in this case related to the four classes we find when Q_3 is a diagonalmatrix. It would be a little bit complicated to investigate this question by means of matrix calculus. It is much easier to study the wave functions (confining ourselves to the case $m = 0$).

If we rotate the $\boldsymbol{k}$-system about one of the axes through $\frac{\pi}{2}$, the moments of inertia in the Hamiltonian will be interchanged. If we for instance rotate about $\boldsymbol{k}_y$, A_1 and A_3 are interchanged. We may now immediately write down the four groups of wave functions in the new system of coordinates. If we express them in terms of the old coordinates we will obtain the four classes for which Q_1 is a diagonal matrix. χ, ϑ are polar coordinates of $\boldsymbol{f}_z$ in the $\boldsymbol{k}$-system and if we put:

$(1a, b, c)$ $\quad \xi = \sin\vartheta\cos\chi, \quad \eta = \sin\vartheta\sin\chi, \quad \zeta = \cos\vartheta,$

ξ, η, ζ will transform as rectangular coordinates. Our wave functions may be expressed as homogeneous polynomials in ξ, η, ζ of degree j. The four groups are distinguished by whether they are even or odd in ξ, η, ζ. We find:

j even

	ξ	η	ζ
$E+$	e	e	e
$E-$	o	o	e
$O+$	e	o	o
$O-$	o	e	o

j odd

	ξ	η	ζ
$E+$	e	e	o
$E-$	o	o	o
$O+$	e	o	e
$O-$	o	e	e

From this table follows at once what happens if the axes of inertia are interchanged:

a. $A_1 \rightleftarrows A_2$.

j even		j odd	
$E+$	$E+$	$E+$	$E+$
$E-$	$E-$	$E-$	$E-$
$O+$	$O-$	$O+$	$O-$
$O-$	$O+$	$O-$	$O+$

b. $A_1 \rightleftarrows A_3$.

j even		j odd	
$E+$	$E+$	$E+$	$O-$
$E-$	$O+$	$E-$	$E-$
$O+$	$E-$	$O+$	$O+$
$O-$	$O-$	$O-$	$E+$

c. $A_2 \rightleftarrows A_3$.

j even		j odd	
$E+$	$E+$	$E+$	$O+$
$E-$	$O-$	$E-$	$E-$
$O+$	$O+$	$O+$	$E+$
$O-$	$E-$	$O-$	$O-$

These results, deduced for $m = 0$, will also hold for arbitrary m, for they express an algebraical property of the H-matrix that is independent of m.

10, 2. The order of the eigenvalues.

The remarkable theorem was proved by Kramers and Ittman:

If $A_3 > A_2$ and $A_3 > A_1$ and if we call:

the eigenvalues of $E+$, $-W_j$, $-W_{j-4}$, $-W_{j-8}$, ...
$W_j < W_{j-4} < W_{j-8} < \ldots .$;
those of $O+$, $-W_{j-1}$, $-W_{j-5}$, ...
$W_{j-1} < W_{j-5} < \ldots .$;

those of $E-$, $-W_{j-2}$, $-W_{j-6}$, ...
$W_{j-2} < W_{j-6} < \ldots .$;
those of $O-$, $-W_{j-3}$, $-W_{j-7}$, ...
$W_{j-3} < W_{j-7} < \ldots .$;

then we have:

$$W_j < W_{j-1} < W_{j-2} < W_{j-3} < W_{j-4} < W_{j-5} < \ldots .$$

For the proof which consists in an application of Sturm's theorem on algebraic equations, the reader is referred to the original paper.

11. Selection rules.

There exists a set of selection rules for the transitions between the four classes.

In K_{i3} only transitions $O \to O$ and $E \to E$ occur. For the matrix elements of the S-representation vanish unless $s_1 = s_2$. Therefore the E_1, E_2 element will vanish unless $u(\vartheta^\lambda, E_1)$ and $u(\vartheta^\lambda, E_2)$ contain $u(\vartheta^\lambda, s)$ with the same s, that is if both belong to E or to O. In the same way:

In K_{i1} and K_{i2} only transitions $O \to E$ and $E \to O$ occur.

But there are also selection rules for transitions between $+$ and $-$ classes. To calculate in which way the $(s_1 \mid F_i(j_1, j_2) \mid s_2)$ are transformed when we introduce the $+$ and $-$ combinations we consider the linear transformations:

$$(1) \qquad \mathcal{F}_i(s \mid S(j_1) \mid E) = \sum_{s'} (s \mid F_i(j_1, j_2) \mid s')(s' \mid S(j_2) \mid E).$$

For $j_1 = j_2$ we have:

$$(2) \qquad \mathcal{F}_3(s \mid E) = s \,.\, (s \mid E).$$

$$(3) \qquad \mathcal{F}_3(-s \mid E) = -s \,.\, (-s \mid E).$$

$$(4) \qquad \mathcal{F}_3[(s \mid E) \pm (-s \mid E)] = 2s[(s \mid E) \mp (-s \mid E)].$$

Only transitions $+ \to -$ and $- \to +$ occur.
For $j \to j - 1$:

$$(5) \qquad \mathcal{F}_3(s, j \mid E) = \sqrt{(j+s)(j-s)}\,(s, j-1 \mid E).$$

(6) $$\mathcal{T}_3(-s, j \mid \mathrm{E}) = \sqrt{(j-s)(j+s)}\,(-s, j-1 \mid \mathrm{E}).$$

(7) $$\mathcal{T}_3[(s, j \mid \mathrm{E}) \pm (-s, j \mid \mathrm{E})] = \sqrt{(j-s)(j+s)}\,.\,[(s, j-1 \mid \mathrm{E}) \pm (-s, j-1 \mid \mathrm{E})].$$

Only transitions $+ \to +$ and $- \to -$ occur. The selection rules for the other components may be found in the same way — this method has to be used if we also want to know the intensities —, but also by using the results of [10, 1]: the $\frac{\pi}{2}$ rotation that interchanges A_3 and A_1, will also interchange K_{i3} and K_{i1} (a + or − sign is of no importance!).

The final result is expressed in the following diagrams:

$j \leftrightarrow j$	$E+$	$E-$	$O+$	$O-$
K_{i1}	↔	↔		
K_{i2}	↔	↔		
K_{i3}	↔		↔	

$j \leftrightarrow j-1$	$E+$	$E-$	$O+$	$O-$
K_{i1}	↔	↔		
K_{i2}	↔	↔		
K_{i3}	↔	↔	↔	↔

12. Two-valued eigenfunctions and the ξ, η, ζ, χ.

Let us drop the condition that our eigenfunctions must be one-valued, but still claim that they depend continously and in a neighbourhood of any position uniquely on position (using as a measure for the distance of two positions the absolute value of the angle of rotation transforming the first position into the second one). Solutions of the wave equation, $\mathcal{H}\psi = \mathrm{E}\psi$, satisfying these conditions, will be called D-functions. A D-function is not necessarily a continuous function of the Eulerian angles: near the normal postion the Eulerian angles do not depend continuously on position. The parameters ξ, η, ζ, χ, [I 5, 2], are continuous and in the neighbourhood of any position one-valued parameters, therefore: D-functions are continuous and in the neighbourhood of any set of values ξ, η, ζ, χ — = "point" — one-valued functions of the ξ_i. Now it follows from the fact that D-functions are one valued functions of the ξ_i in a neighbourhood of every point, that they are one-valued functions throughout. For the domain of possible values ξ_i is a three dimensional sphere in four dimensional space and in this domain every closed curve can be contracted into one point; as a D-function must return to its initial value when we describe a closed curve in ξ-space that is sufficiently small and as every closed curve can be transformed continuously into a curve as small as we like, a D-function must return to its initial value when we describe any closed curve in ξ-space. D-functions are continuous and one-valued in ξ-space. As ξ, η, ζ, χ, and $-\xi$, $-\eta$, $-\zeta$, $-\chi$ belong to the same position, D-functions are either one-valued or two-valued functions of position; a D-function will be a one-valued function of position and therefore an ordinary eigenfunction, if it is an even function of ξ_i:

$$f(\xi, \eta, \zeta, \chi) = f(-\xi, -\eta, -\zeta, -\chi).$$

12, 1. The wave equation in terms of the ξ_i.

We confine ourselves to a spherical body: $A_1 = A_2 = A_3$. To find the expressions for the operators $\mathcal{Q}_i$ we make use of their geometrical interpretation, [8]. When we carry out a rotation through ε about $\boldsymbol{k}_1$ the ξ_i are increased by:

(1) $d\chi = -\frac{1}{2}\varepsilon\xi; \quad d\xi = \frac{1}{2}\varepsilon\chi; \quad d\eta = \frac{1}{2}\varepsilon\zeta; \quad d\zeta = -\frac{1}{2}\varepsilon\eta.$

(These formulae are obtained by applying [I, 5,1 (5)] with $\chi_1 = 1$, $\xi_1 = \frac{1}{2}\varepsilon$, $\eta_1 = \zeta_1 = 0$). It follows:

(2a) $$\mathcal{Q}_1 = -\tfrac{1}{2}ih\Big[-\xi\frac{\partial}{\partial\chi} + \chi\frac{\partial}{\partial\xi} + \zeta\frac{\partial}{\partial\eta} - \eta\frac{\partial}{\partial\zeta}\Big].$$

In the same way:

(2b) $$\mathcal{Q}_2 = -\tfrac{1}{2}ih\Big[-\eta\frac{\partial}{\partial\chi} + \chi\frac{\partial}{\partial\eta} + \xi\frac{\partial}{\partial\zeta} - \zeta\frac{\partial}{\partial\xi}\Big],$$

(2c) $$\mathcal{Q}_3 = -\tfrac{1}{2}ih\Big[-\zeta\frac{\partial}{\partial\chi} + \chi\frac{\partial}{\partial\zeta} + \eta\frac{\partial}{\partial\xi} - \xi\frac{\partial}{\partial\eta}\Big].$$

Using these expressions we find:

$$(3)\quad \frac{1}{2A}\Big[\sum_i \mathcal{Q}_i^2\Big] = -\frac{h^2}{8A}\Big[\Big(\xi^2+\eta^2+\zeta^2\Big)\frac{\partial^2}{\partial\chi^2} + \Big(\eta^2+\zeta^2+\chi^2\Big)\frac{\partial^2}{\partial\xi^2} + \Big(\zeta^2+\chi^2+\xi^2\Big)\frac{\partial^2}{\partial\eta^2} + \Big(\chi^2+\xi^2+\eta^2\Big)\frac{\partial^2}{\partial\zeta^2} - 3\Big(\xi\frac{\partial}{\partial\xi} + \eta\frac{\partial}{\partial\eta} + \zeta\frac{\partial}{\partial\zeta} + \chi\frac{\partial}{\partial\chi}\Big) - 2\Big(\xi\chi\frac{\partial}{\partial\xi}\frac{\partial}{\partial\chi} + \xi\eta\frac{\partial}{\partial\xi}\frac{\partial}{\partial\eta} + \xi\zeta\frac{\partial}{\partial\xi}\frac{\partial}{\partial\eta} + \eta\zeta\frac{\partial}{\partial\eta}\frac{\partial}{\partial\zeta} + \eta\chi\frac{\partial}{\partial\eta}\frac{\partial}{\partial\chi} + \zeta\chi\frac{\partial}{\partial\zeta}\frac{\partial}{\partial\chi}\Big)\Big].$$

If we call $\mathcal{L}$ the term within the square brackets on the right, the Schrödinger equation becomes:

(4) $$\mathcal{L}\psi + \lambda\psi = 0,$$

where

(5) $$\lambda = \frac{8A}{h^2}\,\mathrm{E}.$$

As $\mathcal{L}$ is invariant under a transformation $\xi_i \to a\xi_i$, the solutions of (4) will be homogeneous in the ξ_i and they will stay solutions belonging to the same value of λ if we drop the condition $\sum_i \xi_i^2 = 1$. We define:

(6) $$r^2 = \xi^2 + \eta^2 + \zeta^2 + \chi^2, \qquad (r > 0),$$

then:

(7) $$\xi\frac{\partial}{\partial\xi} + \eta\frac{\partial}{\partial\eta} + \zeta\frac{\partial}{\partial\zeta} + \chi\frac{\partial}{\partial\chi} = r\frac{\partial}{\partial r},$$

where the differentiation with respect to r must be performed, while the ratio's $\xi : \eta : \zeta : \chi$ remain the same.

$$(8)\quad \frac{1}{r}\frac{\partial}{\partial r}r^3\frac{\partial}{\partial r} = r\frac{\partial}{\partial r}r\frac{\partial}{\partial r} + 2r\frac{\partial}{\partial r} = \Big(\xi\frac{\partial}{\partial\xi} + \eta\frac{\partial}{\partial\eta} + \zeta\frac{\partial}{\partial\zeta} + \chi\frac{\partial}{\partial\chi}\Big)^2 + 2\Big(\xi\frac{\partial}{\partial\xi} + \eta\frac{\partial}{\partial\eta} + \zeta\frac{\partial}{\partial\zeta} + \chi\frac{\partial}{\partial\chi}\Big) = \Big(\xi^2\frac{\partial^2}{\partial\xi^2} + \eta^2\frac{\partial^2}{\partial\eta^2} + \zeta^2\frac{\partial^2}{\partial\zeta^2} + \chi^2\frac{\partial^2}{\partial\chi^2}\Big) + 3\Big(\xi\frac{\partial}{\partial\xi} + \eta\frac{\partial}{\partial\eta} + \zeta\frac{\partial}{\partial\zeta} + \chi\frac{\partial}{\partial\chi}\Big) + 2\Big(\xi\eta\frac{\partial}{\partial\xi}\frac{\partial}{\partial\eta} + \xi\chi\frac{\partial}{\partial\xi}\frac{\partial}{\partial\chi} + \xi\zeta\frac{\partial}{\partial\xi}\frac{\partial}{\partial\zeta} + \zeta\eta\frac{\partial}{\partial\zeta}\frac{\partial}{\partial\eta} + \zeta\xi\frac{\partial}{\partial\zeta}\frac{\partial}{\partial\xi} + \zeta\chi\frac{\partial}{\partial\zeta}\frac{\partial}{\partial\chi}\Big).$$

Consequently:

(9) $$\mathcal{L} = r^2\Big(\frac{\partial^2}{\partial\xi^2} + \frac{\partial^2}{\partial\eta^2} + \frac{\partial^2}{\partial\zeta^2} + \frac{\partial^2}{\partial\chi^2}\Big) - \frac{1}{r}\frac{\partial}{\partial r}r^3\frac{\partial}{\partial r}.$$

This shows: the eigenfunctions of our equation are homogeneous harmonic polynomials. For if $P(\xi)$ is such a polynomial of degree n we have:

(10) $$\mathcal{L}P = -n(n+2)P,$$

and

$$\mathrm{E} = \frac{h^2}{2\mathrm{A}}\cdot\frac{n}{2}\Big(\frac{n}{2}+1\Big).$$

$\frac{n}{2}$ corresponds to the quantum number j.

Also the eigenfunctions for an assymetric body are eigenfunctions of $\sum \mathcal{Q}_i^2$, for $\sum_i \mathrm{Q}_i^2$ is a diagonalmatrix (see [6]). We have thus ar-

rived at the general result: D-functions are homogeneous harmonic polynomials in four dimensional space. The functions with even n are the ordinary (one-valued) wavefunctions, those for which n is odd the two-valued wave functions. That the harmonic polynomials form a complete orthogonal set on a sphere with radius unity is a well known result of the theory of potential.

III.

REPRESENTATION OF THE GROUP OF THREE-DIMENSIONAL ROTATIONS.

1. One- and two-valued representations.

If to every rotation R there corresponds a matrix $P(R)$ and if to the product of two rotations there corresponds the product of the matrices, $P(R_2)P(R_1) = P(R_2R_1)$, then the $P(R)$ are said to form a *matrix representation* of the rotationgroup. The problem is to find all irreducible representations. The construction of other representations is then trivial.

From the matrix elements of the representations we claim that they depend continuously and in the neighbourhood of any rotation uniquely on the rotations (or, once a normal position of a rigid body has been fixed, on the positions). It follows [II, 12]: the matrix elements are continuous and one-valued functions of the ξ_l. This condition also admits two valued representations: to every rotation correspond two matrices, $P_1(R)$, $P_2(R)$ and $P_i(R_2) \,.\, P_k(R_1)$ is either $= P_1(R_2R_1)$ or $= P_2(R_2R_1)$. But any representation has to be a one-valued representation of the group formed by the quaternions $\chi + \xi j + \eta k + \zeta l$.

The conclusions of [II, 12] were based on the fact that ξ-space is simply connected. Any closed curve in ξ-space may be contracted into one point. To such a closed curve in ξ-space there corresponds a continuous sequence of positions, the final and initial position being the same; a closed motion, we may say. To the contracting of the ξ-curve into a point corresponds a continuous changing of our closed motion, until the body remains

at rest, while the motion always remains closed. Not every closed motion can, however, be "contracted into rest": To a curve connecting ξ, η, ζ, χ with $-\xi, -\eta, -\zeta, -\chi$ there corresponds a closed motion that cannot be contracted; it may be changed into a rotation through 2π. Accordingly we may say: the two-valuedness of the ξ_l, the existence of D-functions, the possibility of two-valued representations, are based on the kinematical fact that a 2π rotation cannot be contracted. A 4π rotation can be contracted, therefore there do not exist more-valued representations.

2. Infinitesimal transformations.

Let $R_i(\varphi)$ be the three dimensional matrix description of a rotation through φ about the i-axis, $P_i(\varphi)$ its representation. If ε is a small quantity we have

$$R_i(\varepsilon) = 1 + \varepsilon D_i + O(\varepsilon^2) \tag{1}$$

(see [I 6]) and for the representation:

$$P_i(\varepsilon) = 1 + \varepsilon N_i + O(\varepsilon^2) \tag{2}$$

where N_i is independent of ε. The N_i's are called infinitesimal transformations. Let us divide φ into n equal parts. We have:

$$P_i(\varphi) = \left\{P_i\left(\frac{\varphi}{n}\right)\right\}^n = \left(1 + \frac{\varphi}{n}N_i\right)^n + O\left(\frac{1}{n}\right) \tag{3}$$

and for $n \to \infty$:

$$P_i(\varphi) = \exp \varphi N_i. \tag{4}$$

The definition

$$\exp(\varphi N_i) = \lim_{n\to\infty}\left(1 + \frac{\varphi}{n}N_i\right)^n \tag{5}$$

may be seen to be equivalent to the definition:

$$\exp(\varphi N_i) = 1 + \varphi N_i + \frac{\varphi^2}{2!}N_i^2 + \ldots. \tag{6}$$

Let us consider the expression:

$$R_1(\varphi)R_2(\varphi)\{R_1(\varphi)\}^{-1}\{R_2(\varphi)\}^{-1}. \tag{7}$$

By developping into series and neglecting powers higher than the second one we find:

$$(1 + \varphi D_1 + \tfrac{1}{2}\varphi^2 D_1^2 + \ldots.)(1 + \varphi D_2 + \tfrac{1}{2}\varphi^2 D_2^2 + \ldots.).$$

$$(1 - \varphi D_1 + \tfrac{1}{2}\varphi^2 D_1^2 + \ldots.)(1 - \varphi D_2 + \tfrac{1}{2}\varphi^2 D_2^2 + \ldots.) = \tag{8}$$
$$= 1 + \varphi^2(D_1D_2 - D_2D_1) + \ldots. = 1 + \varphi^2 D_3.$$

In the same way we find for the representations:

$$P_1(\varphi)P_2(\varphi)P_1(-\varphi)P_2(-\varphi) = 1 + \varphi^2(N_1N_2 - N_2N_1) + \ldots. \tag{9}$$

On the other hand $1 + \varepsilon D_3$ is represented by $1 + \varepsilon N_3$ therefore:

$$N_1N_2 - N_2N_1 = N_3. \tag{10a}$$

In the same way:

$$N_2N_3 - N_3N_2 = N_1, \tag{10b}$$

$$N_3N_1 - N_1N_3 = N_2. \tag{10c}$$

2,1. Algebraical construction of the irreducible representations.

It follows from [II 5] that the irreducible sets of matrices, satisfying [2 (10)], are given by:

$$N_i = -iM_i(j). \tag{1}$$

We will show that to every j corresponds one irreducible representation having $-iM_i(j)$ as infinitesimal transformations.

Consider the transformation:

$$M_k^* = \sum_m T_{km}M_m = (1 + \varepsilon i M_l)M_k(1 - \varepsilon i M_l). \tag{2}$$

It is, with an error $O(\varepsilon^2)$, a rotation through the angle ε about the l-axis. More general the transformation

$$M_l^* = (1 + \varepsilon i \sum_k a_k M_k)M_l(1 - \varepsilon i \sum_k a_k M_k) \tag{3}$$

is, with an error $O(\varepsilon^2)$, a rotation through ε about the axis a_1, a_2, a_3.

For a finite rotation we may again divide the angle into n equal parts and by a reasoning similar to that of [2] we find: the transformation

$$M_l^* = \exp(+i\varphi \,.\, \sum_k a_k M_k) \,.\, M_l \,.\, \exp(-i\varphi \sum_k a_k M_k) \tag{4}$$

is a rotation through φ about a_1, a_2, a_3.

$$\exp\left(-i\varphi \sum_k a_k M_k\right) = \lim_{n\to\infty}\left(1 - i\frac{\varphi}{n}\sum_k a_k M_k\right)^n = \tag{5}$$
$$= 1 - i\varphi \sum_k a_k M_k - \tfrac{1}{2}\varphi^2\Big\{\sum_k a_k M_k\Big\}^2 - \ldots .$$

The matrices

$$L(\varphi, a_k) = \| \exp\left(-i\varphi \sum a_k M_k\right) \| \tag{6}$$

are unitary. For

$$\left(1 - i\frac{\varphi}{n}\sum a_k M_k\right)$$

is unitary with an error $O(n^{-2})$, therefore

$$\left(1 - i\frac{\varphi}{n}\sum a_k M_k\right)^n$$

is unitary with an error $O(n^{-1})$ and the limit for $n \to \infty$ will be unitary.

$$\mathrm{Det} \| \exp\left(-i\varphi \sum a_k M_k\right) \| = 1 \tag{7}$$

for

$$\mathrm{Det} \| 1 - i\frac{\varphi}{n}\sum a_k M_k \| = 1 - i\frac{\varphi}{n}\,\mathrm{Sp}\{\sum a_k M_k\} + O\left(\frac{1}{n^2}\right) = \tag{8}$$
$$= 1 + O\left(\frac{1}{n^2}\right).$$

(Here $\mathrm{Sp} \sum a_k M_k$ means the sun of the diagonal elements, which vanishes.)

Further $L(\varphi, a_k)$ depends continuously and in a neighbourhood of any rotation uniquely on the rotations and is therefore a continuous one-valued function of the ξ, η, ζ, χ: $L(\xi_l)$.

We will show that the $L(\xi_k)$ form a representation. Let us consider two transformations

$$\sum_k R(\xi)^k_l M_k = L(\xi)^{-1} \,.\, M_l \,.\, L(\xi). \tag{9a}$$

$$\sum_k R(\xi')^k_l M_k = L(\xi')^{-1} \,.\, M_l \,.\, L(\xi'). \tag{9b}$$

We have:

$$\sum_{l,m} R(\xi')^l_k \,.\, R(\xi)^m_l \,.\, M_m = \{L(\xi') \,.\, L(\xi)\}^{-1} M_k \,.\, L(\xi') \,.\, L(\xi). \tag{10}$$

On the other hand, if the resultant rotation is given by ξ'':

$$\sum_m R(\xi'')^m_k M_m = L(\xi'')^{-1} \,.\, M_k \,.\, L(\xi'). \tag{11}$$

It follows:

$$L(\xi') \,.\, L(\xi) = L(\xi'') \,.\, c \tag{12}$$

when c is an ordinary (complex) number; for only a matrix proportional unity commutes with all $M_l(j)$ and from (10) and (11) it follows that

$$L(\xi'')^{-1} \,.\, L(\xi') \,.\, L(\xi)$$

has this property.
As $\mathrm{Det} \| L(\xi) \| = 1$ for all ξ, it follows:

$$\mathrm{Det} \| c \| = c^{2j+1} = 1. \tag{13}$$

Further it may easily be verified that for infinitesimal transformations $L(\xi)$, $L(\xi')$, one has to take $c = 1$. By changing ξ, ξ' continuously one infers that $c = 1$ for any ξ, ξ'. We have thus proved:

If $R(\xi') \,.\, R(\xi) = R(\xi'')$ then $L(\xi') \,.\, L(\xi) = L(\xi'')$. The $L(\xi)$ form a representation.

That the representation is irreducible follows from the fact that already the $M_l(j)$ form an irreducible set.

The irreducible representations constructed in this section will be called M-representations.

2, 2. The case $j = \frac{1}{2}$.

Apart from the trivial $j = 0$ (in which case all M_l are zero and the representations simply the number 1) the simplest possible example is afforded by taking $j = \frac{1}{2}$. If we write

$$-iM_l(\tfrac{1}{2}) = \tfrac{1}{2}k_l, \tag{1}$$

we have:

$$(2a,b,c)\quad k_3 = \begin{Vmatrix} -i & 0 \\ 0 & +i \end{Vmatrix};\quad k_1 = \begin{Vmatrix} 0 & -i \\ -i & 0 \end{Vmatrix};\quad k_2 = \begin{Vmatrix} 0 & -1 \\ +1 & 0 \end{Vmatrix}.$$

The k_l satisfy the relations:

(3) $$k_1k_2 = -k_2k_1 = k_3 \quad \text{and so on,}$$

(4) $$k_1^2 = k_2^2 = k_3^2 = -1,$$

just the relations satisfied by the quaternions, [I 5]. The series:

$$1 + \frac{\varphi}{2}\left(\sum_k a_k k_k\right) + \frac{1}{2!}\left(\frac{\varphi}{2}\right)^2\left(\sum_k a_k k_k\right)^2 + \ldots .$$

may now easily be summed; we find:

(5) $$L(\xi) = \cos\frac{\varphi}{2} + \sin\frac{\varphi}{2}\sum_k a_k k_k = \chi + \xi k_1 + \eta k_2 + \zeta k_3.$$

That the transformation

(6) $$k_l^* = (\cos\frac{\varphi}{2} - \sin\frac{\varphi}{2}\sum_k a_k k_k) k_l (\cos\frac{\varphi}{2} + \sin\frac{\varphi}{2}\sum_k a_k k_k)$$

is an orthogonal transformation was already shown in [I 5,1]. It appears here as a special case of our general theory. (In [I] we used a different sign: we were there interested not in the transformation of the k_l but in the transformation of the coefficients r_l in the expression $\sum_l r_l \,.\, k_l$). It may be seen that any two dimensional unitary matrix with determinant $+1$ may be written in the form:

(7) $$u(\xi) = \chi + \xi k_1 + \eta k_2 + \zeta k_3$$

with $\sum \xi_l^2 = 1$.

2,3. The general case; one- and two-valued representations. In the general case we at once obtain a closed expression for the representation of the rotations about the z axis:

(1) $$P_z(\varphi) = \begin{Vmatrix} e^{-ij\varphi} & 0 & & & & \\ 0 & e^{-i(j-1)\varphi} & & & & \\ & & \ddots & & & \\ & & & 1 & & \\ & & & & e^{+i(j-1)\varphi} & 0 \\ & & & & 0 & e^{+ij\varphi} \end{Vmatrix}.$$

From this formula we can draw an important conclusion. For j integer the matrixelements are one-valued functions of the rotations, for j half an odd integer however, they are two-valued.

If follows further from [I 4] that the representations depend on the Eulerian angles in the following way:

(2) $$\| P_{ms}(\vartheta^\lambda) \| = \begin{Vmatrix} e^{-ij\psi} & & & \\ & \ddots & & \\ & & & e^{ij\psi} \end{Vmatrix} \| f_{ms}(\vartheta) \| \begin{Vmatrix} e^{-ij\varphi} & & & \\ & \ddots & & \\ & & & e^{ij\varphi} \end{Vmatrix}.$$

(3) $$P_{ms}(\vartheta^\lambda) = e^{-im\psi}\, e^{-is\varphi}\, f_{sm}(\vartheta).$$

An explicit expression for $f_{sm}(\vartheta)$ may be found but we will not discuss this question.

3. Differentialequations satisfied by the representations. Any representation $\| P_{sm}(R) \|$ satisfies the equation:

(1) $$P_{sm}(R_2R_1) = \sum_n P_{sn}(R_2)P_{nm}(R_1).$$

Let now R_2 be an infinitesimal rotation:

(2) $$R_2 = 1 + \varepsilon D_i.$$

Then we have:

(3) $$P_{sm}((1 + \varepsilon D_i) \,.\, R_1) - P_{sm}(R_1) = \varepsilon \sum_n (N_i)_{sn} P_{nm}(R_1).$$

If R_2 is described by ϑ^ν, $(1 + \varepsilon D_i)\, R_2$ will be described by $\vartheta^{*\nu} = \vartheta^\nu + \varepsilon p_i^\nu$, consequently:

(4) $$p_i^\nu \frac{\partial}{\partial \vartheta^\nu} \,.\, P_{sm}(\vartheta^\lambda) = \sum_n (N_i)_{sn} P_{nm}(\vartheta^\lambda).$$

Assuming that R_1 is infinitesimal we find:

(5) $$q_i^\nu \frac{\partial}{\partial \vartheta^\nu} \,.\, P_{sm}(\vartheta^\lambda) = \sum_n (N_i)_{nm} \,.\, P_{sn}(\vartheta^\lambda).$$

If $\| P_{sn} \|$ is one of the M-representations, we have:

(6) $$(N_i)_{sn} = -iM(j)_{sn}$$

or, taking the conjugate complex of (4) and (5) and multiplying by i:

$$(7) \qquad -ip_i^\nu \frac{\partial}{\partial \vartheta^\nu} \overline{\mathrm{P}}_{sm}(\vartheta^\lambda) = \sum_n \mathrm{M}_{ns} \overline{\mathrm{P}}_{nm}(\vartheta^\lambda).$$

$$(8) \qquad -iq_i^\nu \frac{\partial}{\partial \vartheta^\nu} \overline{\mathrm{P}}_{sm}(\vartheta^\lambda) = \sum_n \overline{\mathrm{M}}_{nm} \overline{\mathrm{P}}_{sn}(\vartheta^\lambda).$$

$$(9) \qquad \sum_i \left[-ip_i^\nu \frac{\partial}{\partial \vartheta^\nu} \right]^2 \overline{\mathrm{P}}_{sm} = j(j+1) \overline{\mathrm{P}}_{sm}.$$

It follows: the conjugate complex of a matrix element of an M-representation $\overline{\mathrm{P}}(\vartheta^\nu; j)_{sm}$ is equal (apart from a constant factor not depending on s, m — it does depend on j, see [IV 8] —) to the eigenfunction belonging to the S-representation.

If we also want to include the two-valued representations we better use the ξ_l. The argument can be repeated using the expressions in terms of the ξ_l (see [II 12, 1]) instead of the $p_i^\nu \frac{\partial}{\partial \vartheta^\nu}$. The $\overline{\mathrm{P}}_{sm}(\xi; j)$ form a set of mutually orthogonal spherical harmonics in four dimensions.

4. Transformation of continuous functions on a sphere.

Let Θ, Φ be polarcoordinates in the f-system. If we carry out a rotation defined by Eulerian angles ϑ^ν, we will have:

$$(1) \qquad \Theta^* = \Theta^*(\Theta, \Phi; \vartheta^\nu),$$

$$(2) \qquad \Phi^* = \Phi^*(\Theta, \Phi; \vartheta^\nu).$$

The transformations $\Theta, \Phi \to \Theta^*, \Phi^*$ form a group isomorphic to the group of rotations, they form a realization of this group.

Let $f(\Theta, \Phi)$ be an arbitrary differentiable one-valued function. We call transformed function, f^*, the function with the property:

$$(3) \qquad f^*(\Theta^*, \Phi^*) = f(\Theta, \Phi).$$

If we write $f^* = \mathcal{T}_R f$ the operators $\mathcal{T}_R$ will multiply in the same order as the rotations. Consider a complete orthogonal set of functions $f_n(\Theta, \Phi)$,

$$(4) \qquad \int_0^{2\pi} \int_0^{\pi} \overline{f_n} f_m \sin\Theta d\Theta d\Phi = \delta_{nm}.$$

Then also the $\mathcal{T}_\mathrm{R} f_n$ will form an orthogonal set, for if f and g are two arbitrary functions, we have:

$$(5) \qquad \int_0^{2\pi} \int_0^{\pi} fg \sin\Theta d\Theta d\Phi = \int_0^{2\pi} \int_0^{\pi} (\mathcal{T}_\mathrm{R} f)(\mathcal{T}_\mathrm{R} g) \sin\Theta d\Theta d\Phi$$

as is seen by introducing Θ^*, Φ^* as variables of integration and remarking that:

$$(6) \qquad \sin\Theta d\Theta d\Phi = \sin\Theta^* d\Theta^* d\Phi^*.$$

It will now be possible to expand $\mathcal{T}_\mathrm{R} f_n$ in terms of the f_m:

$$(7) \qquad \mathcal{T}_\mathrm{R} f_n = \sum_m \mathrm{T(R)}_{mn} f_m.$$

It follows from the general relation between operators and matrices, that the $\| \mathrm{T(R)}_{mn} \|$ will form a representation of our group. $\| \mathrm{T(R)}_{mn} \|$ is a unitary matrix, for:

$$(8) \qquad \begin{aligned} \iint (\overline{\mathcal{T}_\mathrm{R} f_n})(\mathcal{T}_\mathrm{R} f_m) &= \sum_{l,k} \overline{\mathrm{T(R)}}_{ln} \cdot \mathrm{T(R)}_{km} \iint \overline{f_l} \cdot f_k = \\ &= \sum_k \overline{\mathrm{T(R)}_{kn}}\, \mathrm{T(R)}_{km} = \delta_{nm}. \end{aligned}$$

By suitably choosing our functions, it will be possible to reduce the T-matrices; the f_n will then be divided into sets transforming with irreducible representations:

$$(9) \qquad f_m(\Theta, \Phi) = \mathcal{T}_\mathrm{R} f_m(\Theta^*, \Phi^*) = \sum \mathrm{P}_{nm}(\vartheta^\nu) f_n(\Theta^*, \Phi^*).$$

As we confine ourselves to one-valued functions, only one-valued representations will occur.

If R is an infinitesimal rotation this becomes:

$$(10) \qquad f_m(\Theta^*, \Phi^*) - f_m(\Theta, \Phi) = \varepsilon^i \sum_n (\mathrm{N}_i)_{nm} f_n(\Theta, \Phi),$$

or:

$$(11) \qquad -\pi_i^\lambda \frac{\partial}{\partial \Theta^\lambda} f_m = \sum_n (\mathrm{N}_i)_{nm} f_n,$$

where

$$\pi_i^\lambda(\Theta) = \operatorname*{Lim}_{\varepsilon \to 0} \frac{\Theta^{*\lambda} - \Theta^\lambda}{\varepsilon}; \tag{12}$$

here $\Theta^{*\lambda}$ is obtained from Θ^λ by a rotation through ε about the i-axis. Multiplying by i we find:

$$-i\Pi_i f_m = -i\pi_i^\lambda \frac{\partial}{\partial \Theta^\lambda} f_m = \sum_n (M_i(j))_{nm} f_n; \tag{13}$$

$$\sum_i (\Pi_i)^2 f_m + j(j+1) f_m = 0. \tag{14}$$

We find:

$$\Pi_1 = -\sin\Phi \frac{\partial}{\partial\Theta} - \cos\Phi \frac{\cos\Theta}{\sin\Theta} \frac{\partial}{\partial\Phi}, \tag{15}$$

$$\Pi_2 = \cos\Phi \frac{\partial}{\partial\Theta} - \sin\Phi \frac{\cos\Theta}{\sin\Theta} \frac{\partial}{\partial\Phi}, \tag{16}$$

$$\Pi_3 = \frac{\partial}{\partial\Phi}, \tag{17}$$

which leads to:

$$\frac{1}{\sin\Theta}\left\{\frac{\partial}{\partial\Theta}\left(\sin\Theta \frac{\partial f_m}{\partial\Theta}\right) + \frac{1}{\sin\Theta}\frac{\partial^2 f_m}{\partial\Phi^2}\right\} + j(j+1) f_m = 0. \tag{18}$$

The functions transforming with an irreducible representation are spherical harmonics of degree j.

4, 1. Transformation of spherical harmonics.

To an integer value j, there will correspond $2j+1$ linearly independant solutions, $Y_m(\Theta, \Phi)$, of [4(18)]. We may choose them orthogonal and normalized, for instance:

(1) $\quad Y_m(\Theta, \Phi) = N(m, j)\, P_j^m(\cos\Theta)\, e^{im\Phi} \quad -j \leqslant m \leqslant j.$

where $N(m, j)$ is a normalization factor. If we carry out a rotation, $Y_m^*(\Theta^*, \Phi^*)$ will be a solution of [4(18)] expressed in terms of the Θ^*, Φ^*. But this equation is invariant, it has exactly the same form in Θ^*, Φ^* as it has in Θ, Φ. Therefore $Y_m^*(\Theta^*, \Phi^*)$ will be a linear combination of the $Y_m(\Theta^*, \Phi^*)$:

(2) $\quad Y_m(\Theta, \Phi) = \mathcal{T}_R Y_m(\Theta^*, \Phi^*) = \sum_n P_{nm} Y_n(\Theta^*, \Theta^*).$

That P_{nm} is an irreducible $(2j+1)$-dimensional representation follows from the fact that the representation of rotations about the z-axis has the correct form, which determines the representation apart from phase-factors.

5. Transformation of the eigenfunctions of a rigid body.

The method of the preceding section may be applied to any invariant equation; we use it to give another proof of the result of [3]. Let $\psi(\vartheta^\nu; j, E, m)$ be a solution of our wave equation. We may express it in terms of Eulerian angles $\vartheta^{*\nu}$ that are obtained from ϑ^ν by a rotation $\vartheta_1{}^\nu$. $\mathcal{T}_R\psi(\vartheta^{*\nu}; j, E, m)$ will be a solution of the wave equation expressed in $\vartheta^{*\nu}$. But this equation has just the same form as the old one, therefore $\mathcal{T}_R\psi(\vartheta^{*\nu}; j, E, m)$ must be a linear combination of the $(2j+1)$ $\psi(\vartheta^{*\nu}; j, E, m)$'s. Therefore:

(1) $\quad \psi(\vartheta^\nu; j, E, m) = \mathcal{T}_R\psi(\vartheta^{*\nu}; j, E, m) = \sum_n P_{nm}(\vartheta_1{}^\nu)\psi(\vartheta^{*\nu}; j, E, n)$

with unitary P_{nm} (the ψ being orthogonal and normalized).

(2) $\quad \psi(\vartheta^{*\nu}; j, E, n) = \sum_m \overline{P}_{nm}(\vartheta_1{}^\lambda) \cdot \psi(\vartheta^\nu; j, E, m).$

Taking for ϑ^ν the values for a rotation zero, it follows:

(3) $\quad \psi(\vartheta_1{}^\nu; j, E, n) = \sum_m \overline{P}_{nm}(\vartheta_1{}^\nu) \cdot \psi(\vartheta_0{}^\lambda; j, E, m).$

Every eigenfunction is a linear combination of matrix-elements. That in the case of a symmetrical body the eigenfunctions belonging to the S-representation are equal to the $\overline{P}_{nm}$ is seen from the way in which they depend on ψ and φ.

If R is an infinitesimal rotation we have

(4) $\quad f(\vartheta^\lambda) - f(\vartheta^{*\lambda}) = \mathcal{T}_R f(\vartheta^{*\lambda}) - f(\vartheta^{*\lambda}) = -\varepsilon \frac{i}{h} \mathcal{P}_i f(\vartheta^{*\lambda}).$

From the equation

$$\mathcal{H} f = \lambda f \tag{5}$$

it follows:

$$\mathcal{H}(1+\varepsilon\frac{i}{h}\mathcal{P}_i)f^*(\vartheta^\lambda)=\lambda(1+\varepsilon\frac{i}{h}\mathcal{P}_i)f^*(\vartheta^\lambda), \tag{6}$$

$$\left[\mathcal{H}-\varepsilon\frac{i}{h}(\mathcal{P}_i\mathcal{H}-\mathcal{H}\mathcal{P}_i)\right]f^*=\lambda f^* \tag{7}$$

and as $\mathcal{P}_i$ commutes with $\mathcal{H}$:

$$\mathcal{H}f^*=\lambda f^*. \tag{8}$$

Since this is true for infinitesimal rotations it is true for any rotation. The invariance of $\mathcal{H}$ and the fact that $\mathcal{P}_i$ commutes with $\mathcal{H}$ (and therefore is an integral) are connected with each other just like in classical theory.

5, 1. Fourdimensional formulation.
The argument of the preceding section may be repeated using the parameters ξ_l instead of the ϑ^ν; we can then also include the two valued representations.

It is worth while to investigate more closely, why the matrix-elements satisfy the four dimensional Laplace equation. If a position is characterised by ξ_l and we carry out a rotation $(\xi_1)_l$ we will have (see [I 5,1])

$$\xi_l^*=\sum_k A_{lk}\xi_k \tag{1}$$

where A_{lk} is a linear function of $(\xi_1)_l$ and satisfies the relations:

$$\sum_m A_{km}A_{lm}=\delta_{kl}. \tag{2}$$

The transformations $\xi\to\xi^*$ form a three-parametric subgroup of the group of fourdimensional rotations. Now the Laplace equation is invariant under any orthogonal transformation, therefore it is invariant under the special transformations $\xi\to\xi^*$ and we may apply the same reasoning as in the case of spherical harmonics on a two dimensional sphere in three dimensional space.

IV.

CONTINUOUS GROUPS AND THEIR REPRESENTATIONS

A. OUTLINE OF THE GENERAL THEORY.

1. Definition of an *r*-parametric continuous group.
In [I, 2] a general definition of a group was given. In order to state when a set of elements will be said to form a continuous group, we first have to introduce the idea of distance between two elements so that it is possible to speak of the *neighbourhood* of an element. If our group is a group of linear transformations (matrices) the sum of the square moduli of the differences of corresponding matrix elements affords a natural measure of distance; more general, if it is a group of transformations of a Euclidean continuum, the distance may be measured by the distances of corresponding points. We now give the definition:

A group is an r-parametric continuous group, $\mathfrak{G}_r$, if it satisfies the conditions:

a. A neighbourhood of any element can be brought in one-to-one-correspondence to an open continuum in r-dimensional Euclidean space. The elements belonging to a neighbourhood of any element may accordingly be characterized by r continuously varying parameters, φ^λ.

b. The group is connected: any two elements may be connected by a continuous curve consisting of elements only.

c. If $S_3=S_2S_1$ and we keep one of the S's fixed, the remaining two elements depend continuously on each other (continuity

may be defined in the usual way as soon as distance is defined).

In this chapter we will especially study groups that are simply connected (any closed curve may be contracted) and closed (all limitpoints of points in $\mathfrak{G}$ belong to $\mathfrak{G}$) and which may be covered by a finite number of parts $\mathfrak{A}_i$ each of which may be brought into one-to-one-correspondence to r parameters taking all values of a finite open region in r-dimensional Euclidean space. The group of quaternions studied in [III] satisfies these conditions.

2. Realizations; the parameter group.

If to every element there corresponds a transformation of a continuum $\mathfrak{C}$ into itself and if these transformations multiply in the same way as the elements, they are said to form a realization. We will only consider continuous realizations that is realizations for which the natural definition of distance falls together with the definition given for the abstract group (often one will start with a realization and then define distance in the abstract group such as to satisfy this condition). For elements $< \mathfrak{A}_i$ the transformation will be given by formulae of the form:

$$x^{*n} = f^n(x^i;\ \varphi^\varrho) \tag{1}$$

where the φ^ϱ's are the parameters belonging to $\mathfrak{A}_i$ and f^n is a continuous function.

One realization of a group is given by the transformations of groupspace into itself: the formula $S^* = S'S$ may be interpreted as a transformation of a point S of group space into S^*; that these transformations form a realization is seen from the formula $S''S^* = (S''S')S$. If $S^* = S'S$ where S belongs to an $\mathfrak{A}_i$ described by φ^λ, S' to an $\mathfrak{A}_k$ described by ψ^ϱ, S^* to an $\mathfrak{A}_l$ described by χ^σ we have for a neighbourhood of these elements:

$$\chi^\varrho = g^\varrho(\psi^\lambda;\ \varphi^\mu) \tag{2}$$

where g^ϱ is a continuous function.

It may be proved: if we have found a set of transformations depending continuously and in a neighbourhood of any transformation uniquely on the elements of a closed, simply connected group they depend continuously and uniquely on the group

throughout and if they form a realization in a neighbourhood of any element (that will say: if $S' = \delta S \,.\, S$, S and S' close to each other, then $P' = \delta P \,.\, P$; analogously for $S' = S \,.\, \delta S$) then they form a realization. It follows: if we have found a realization of a neighbourhood of unity of a simply connected group we can construct a realization of the whole of our group by multiplication.

The most important realizations are realizations by linear transformations; we call them representations.

3. Lie-groups.

If the functions g^ϱ of [2(2)] possess first and second derivatives with respect to all arguments, the group will be called an (abstract) L(ie)-group; if the f^i of [2(1)] have this property we speak of an L-group of transformations. For L-groups it is possible — just as in the case of three dimensional rotations — to introduce the notion of infinitesimal transformations and to reduce the problem of finding all irreducible representations to the algebraïcal problem of finding representations for a finite number of quantities. The problem arises whether any closed, simply connected continuous group is an L-group; as far as I know no answer on this question has been given.

4. Lie's first theorem first part. Infinitesimal transformations.

Consider an L-group of transformations:

$$x^{*i} = f^i(x^n;\ \varphi^\varrho). \tag{1}$$

One can prove:

$$\frac{\partial x^{*i}}{\partial \varphi^\varrho} = c^\lambda_\varrho(\varphi)\mathrm{U}^i_\lambda(x^*), \tag{2}$$

with

$$\mathrm{Det}\ \| c^\varrho_\lambda(\varphi) \| \neq 0. \tag{3}$$

For the element unity we have:

$$c^\varrho_\lambda(\mathrm{E}) = \delta^\varrho_\lambda. \tag{4}$$

The c_λ^ϱ depend on the constitution of the abstract group only

The U_λ^i are called infinitesimal transformations. Indeed a transformation in the neighbourhood of unity will be given by:

(5) $$x^{*i} - x^i = \delta\varphi^\lambda U_\lambda^i(x).$$

Symbolically (1) may be written:

(6) $$x^* = S(\varphi^\varrho)x,$$

and (5):

(7) $$x^* - x = \delta\varphi^\lambda U_\lambda x$$

(2) gets:

(8) $$S(\varphi^\varrho + \delta\varphi^\varrho)x = (1 + \delta\varphi^\varrho c_\varrho^\lambda(\varphi)U_\lambda) \,.\, S(\varphi^\varrho)x$$

or:

(9) $$S(\varphi^\varrho + \delta\varphi^\varrho)S(\varphi^\varrho)^{-1} = (1 + \delta\varphi^\varrho c_\varrho^\lambda(\varphi)U_\lambda.$$

This symbolism gets a less abstract meaning in the (most important) case that $S(\varphi)$ (and consequently also U_λ) is a matrix.

The transformation $S(\varphi^\varrho)^{-1}S(\varphi^\varrho + \delta\varphi^\varrho)$ will also be a linear combination of the U_λ:

(10) $$S(\varphi^\varrho)^{-1}S(\varphi^\varrho + \delta\varphi^\varrho) = (1 + \delta\varphi^\varrho a_\varrho^\lambda(\varphi)U_\lambda$$

which is the symbolical formulation of:

(11) $$f^i(x^n;\ \varphi^\varrho + \delta\varphi^\varrho) = f^i(x^n + \delta\varphi^\varrho a_\varrho^\lambda(\varphi)U_\lambda^n(x);\ \varphi^\varrho).$$

An example is given by the theory of three dimensional rotations. If φ^ϱ are the Eulerian angles, S the three dimensional orthogonal matrix, then U_λ will correspond to D_i and c_ϱ^λ and a_ϱ^λ will be the components of the infinitesimal rotation bringing a rigid body from the position φ^ϱ into the position $\varphi^\varrho + \delta\varphi^\varrho$, in the ***f***- and ***k***-system respectively.

If our realization is the parametergroup, (2) becomes (see [2]):

(12) $$\frac{\partial\chi^\varrho}{\partial\psi^\lambda} = d_\mu^\varrho(\chi)\,c_\lambda^\mu(\psi).$$

If the φ^λ's take the values corresponding to unity $\chi^\varrho = \psi^\varrho$ and

(13) $$\delta_\lambda^\varrho = d_\mu^\varrho(\chi)c_\lambda^\mu(\chi).$$

(9) may also be formulated as follows:

(14) $$(1 + \delta\varphi^\lambda U_\lambda) \,.\, S(\varphi^\varrho) = S(\varphi^\varrho + d_\lambda^\varrho(\varphi)\delta\varphi^\lambda).$$

4, 1. Lie's first theorem, second part. Realizations.

One can prove:

If a set of functions $x^{*i} = f^i(x, \varphi)$ satisfy the equations [4(1)] the transformations $x \to x^*$ form a group.

The finite transformations belonging to a neighbourhood of unity can be deduced from the infinitesimal ones in the following way. Write:

(1) $$x^{*i} = x^i + \frac{\varphi^\lambda}{n} U_\lambda^i(x),$$

apply this operation n times and let then n go to infinity; symbolically we may write:

(2) $$x^* = \exp(\varphi^\lambda U_\lambda)x.$$

If $U_\lambda^n(x)$ is a linear function the exponential may also be calculated by using the power series.

The problem arises whether the infinitesimal transformations completely determine a group. As mentioned in [2] a realization of a neighbourhood of unity of a simply connected group determines a realization uniquely. But the infinitesimal transformations determine a neighbourhood of unity: *a realization is determined by its infinitesimal elements*. Two simply connected abstract groups having the same infinitesimal elements $d_\mu^\lambda(\varphi)$ are identical.

5. Lie's second theorem.

If we start out with an arbitrary set of functions, $U_\lambda^n(x)$, we will of course in general not arrive at a group: the differential equations will not be integrable.

A set of functions $U_\lambda^n(x)$ may be regarded as infinitesimal transformations of a continuous group if and only if:

(1) $$\frac{\partial}{\partial x^n}\left(U_\lambda^m(x)\right)U_\nu^n(x) - \frac{\partial}{\partial x^n}\left(U_\nu^m(x)\right)U_\lambda^n(x) = c_{\lambda\nu}{}^\mu U_\mu^m(x)$$

where the $c_{\lambda\nu}{}^\mu$ are constants.
One often writes:

(2) $$(U_\lambda,\ U_\nu) = c_{\lambda\nu}{}^\mu U_\mu;$$

the symbol (U_λ, U_ν) is called a Lie Bracket.

If we call $\mathcal{U}_\lambda$ the differential operator

(3) $$\mathcal{U}_\lambda = -\ U_\lambda^n(x)\frac{\partial}{\partial x^n}$$

we have:

(4) $$\mathcal{U}_\lambda\mathcal{U}_\nu - \mathcal{U}_\nu\mathcal{U}_\lambda = c_{\lambda\nu}{}^\mu\mathcal{U}_\mu.$$

The corresponding operator for the parametergroup will be called $\mathcal{D}_\lambda$:

(5) $$\mathcal{D}_\lambda = -\ d_\lambda^\mu(\varphi)\frac{\partial}{\partial\varphi^\mu}.$$

If $U_\lambda^n(x)$ is a linear function, $U_\lambda^n(x) = (M_\lambda)_m^n \,.\, x^m$ (1) gets:

(6) $$M_\lambda M_\nu - M_\nu M_\lambda = c_{\lambda\nu}{}^\mu M_\mu.$$

In this form the theorem was used in the preceding chapter. The non-vanishing $c_{\lambda\nu}{}^\mu$ were there:

$$c_{12}{}^3 = -\ c_{21}{}^3 = 1$$
$$c_{23}{}^1 = -\ c_{32}{}^1 = 1$$
$$c_{31}{}^2 = -\ c_{13}{}^2 = 1.$$

Together with this theorem one can prove: If for two sets of infinitesimal transformations the constants $c_{\lambda\nu}{}^\mu$ are the same, the groups are isomorphic to each other in a neighbourhood of unity. It follows: if the $c_{\lambda\nu}{}^\mu$'s belong to a simply connected group, a set of infinitesimal transformations satisfying (1) determines a realization. A representation is determined by a set of matrices satisfying (6).

6. Lie's third theorem.

A set of numbers $c_{\lambda\nu}{}^\mu$ defines a group if and only if:

(1) $$c_{\lambda\nu}{}^\mu = -\ c_{\nu\lambda}{}^\mu.$$

(2) $$c_{\alpha\beta}{}^\mu \,.\, c_{\gamma\mu}{}^\varrho + c_{\beta\gamma}{}^\mu \,.\, c_{\alpha\mu}{}^\varrho + c_{\gamma\alpha}{}^\mu \,.\, c_{\beta\mu}{}^\varrho = 0.$$

7. Semi-simple groups.

One may now first try to find all possible sets of $c_{\lambda\nu}{}^\mu$'s. Next one will investigate the topological structure of abstract groups belonging to these constants. And finally one will try to find realizations especially representations by linear transformations.

The theory has mainly been developped for so called semi-simple groups. We will not give the ordinary definition of semi-simple, but a condition that is necessary and sufficiant and therefore may be used as a definition:

A group is semi-simple if and only if the determinant of the quadratic form

(1) $$g_{\lambda\mu} = c_{\lambda\nu}{}^\varrho c_{\varrho\mu}{}^\nu$$

does not vanish, so that there exists a $g^{\lambda\mu}$. The group of three dimensional rotations has this property: we find $g_{\lambda\mu} = \delta_{\lambda\mu}$.

A classification of all semi-simple groups was given by Killing and Cartan.

As to topological structure, it has been proved by Weyl: to any semi-simple set of infinitesimal transformations belongs a closed and simply connected group. It would be incorrect to say: any semi-simple group is simply connected. The most interesting cases are those in which the group is defined "macroscopically", for example as the group of rotations in n-dimensional Euclidean space. From the example of three dimensional rotations we see that such group is not necessarily simply connected, allthough the group is semi-simple. But in any case there will exist an "Uberlagerungs" group (the group of quaternions for the three dimensional rotations) in which any element occurs a finite number of times, that is simply connected. For groups that are not simply connected there will exist manyvalued representations.

The problem of constructing the irreducible representations of all semi-simple groups was treated by Cartan and Weyl.

8. The element of volume.

For the formulation of many general theorems on the representations of continuous groups, it is necessary to introduce the notion of integration over group space. In order to define integration we have to define an element of volume; we have to give a weight to the elements $S(\varphi^\varrho + \vartheta_\varrho \delta\varphi^\varrho)$ where $0 \leqslant \vartheta_\varrho \leqslant 1$. It is possible to do it in such a way that the element of volume is invariant under multiplication on the left and on the right: the weight of the elements $S(\varphi^\varrho + \vartheta_\varrho \delta\varphi^\varrho)$ is equal to that of the elements $TS(\varphi^\varrho + \vartheta_\varrho \delta\varphi^\varrho)$ and also to that of the elements $S(\varphi^\varrho + \vartheta_\varrho \delta\varphi^\varrho)T$.

That the element of volume $\sin\vartheta d\vartheta d\varphi d\psi$ used in the case of three dimensional rotations has this property follows from its geometrical meaning (see [II 2,2]); in the general case the definition is analogous.

We have (see [4 (10)]):

$$(1)\quad S(\varphi)^{-1}S(\varphi^\varrho + \delta\varphi^\varrho) = \{TS(\varphi)\}^{-1}TS(\varphi^\varrho + \delta\varphi^\varrho) = (1 + \delta\varphi^\varrho a_\varrho^\lambda(\varphi)U_\lambda.$$

The expression

$$(2)\qquad \left|\operatorname{Det} \| a_\varrho^\lambda(\varphi) \|\right| . \Pi\delta\varphi^\nu$$

will accordingly be invariant under multiplication on the left. In the same way

$$(3)\qquad \left|\operatorname{Det} \| c_\varrho^\lambda(\varphi) \|\right| . \Pi\delta\varphi^\nu$$

will be invariant under multiplication on the right. Now one can prove that for closed groups:

$$(4)\qquad \left|\operatorname{Det} \| a_\varrho^\lambda(\varphi) \|\right| = \left|\operatorname{Det} \| c_\varrho^\lambda(\varphi) \|\right|.$$

The element of volume:

$$(5)\quad V(\varphi) . \Pi\varphi^\nu = \left|\operatorname{Det} \| a_\varrho^\lambda(\varphi) \|\right| . \Pi\delta\varphi^\nu = \left|\operatorname{Det} \| c_\varrho^\lambda(\varphi) \|\right| . \Pi\delta\varphi^\nu$$

has the required properties. Our conditions determine the element of volume uniquely apart from a constant factor, that may be chosen such as to make the total volume of our group = 1.

One can now prove a number of theorems that are generalizations of well known theorems on finite groups.

A. Any representation is equivalent to a unitary one. If a set of matrices $\| P(S)_{nm} \|$ form a representation then there exists a matrix T such that $TP(S)T^{-1}$ is unitary for all S.

B. If $\| P(S)_{nm} \|$ is an irreducible representation then

$$\int_{\mathfrak{G}} \overline{P(S)}_{nm} . P(S)_{kl} = \delta_{nk} . \delta_{ml} . \frac{1}{d},$$

where d is the dimension of the representation.

C. If $\| P(S)_{nm} \|$, $\| R(S)_{kl} \|$ are two different irreducible representations then:

$$\int_{\mathfrak{G}} P(S)_{nm} . R(S)_{kl} = 0.$$

The matrix elements of the irreducible unitary representations form an orthogonal set. It has been proved by Peter and Weyl: *they form a complete orthogonal set.*

B. A PARTIAL DIFFERENTIALEQUATION BELONGING TO A SEMI-SIMPLE GROUP.

9. Theorem I.

If a differentialoperator $\mathscr{H} = h^{\lambda\mu}\mathscr{D}_\lambda\mathscr{D}_\mu$ commutes with all $\mathscr{D}_\varrho$, then the matrixelements of the irreducible representations are eigenfunctions of $\mathscr{H}$.

Proof.

Any representation satisfies the equation:

$$(1)\qquad P_{nm}(\varphi^\varrho + d_\mu^\varrho \delta\psi^\mu) = \sum_s (1 + \delta\psi^\mu M_\mu)_{ns} . P_{sm}(\varphi^\varrho)$$

where the M_λ's are the infinitesimal elements. (See [4 (14)]). It follows:

$$(2)\qquad -\mathscr{D}_\mu P_{nm} = \sum_s (M_\mu)_{ns} . P_{sm}.$$

(3) $$\mathcal{H}\mathrm{P}_{nm} = \sum_s (h^{\lambda\mu}\mathrm{M}_\mu\mathrm{M}_\lambda)_{ns} \,.\, \mathrm{P}_{sm}.$$

(4) $$0 = (\mathcal{D}_\varrho\mathcal{H} - \mathcal{H}\mathcal{D}_\varrho)\mathrm{P}_{nm} = \sum_s \{(h^{\lambda\mu}\mathrm{M}_\mu\mathrm{M}_\lambda)\mathrm{M}_\varrho - \mathrm{M}_\varrho(h^{\lambda\mu}\mathrm{M}_\mu\mathrm{M}_\lambda)\}_{ns} \,.\, \mathrm{P}_{sm}.$$

(5) $$(h^{\lambda\mu}\mathrm{M}_\mu\mathrm{M}_\lambda)\mathrm{M}_\varrho - \mathrm{M}_\varrho(h^{\lambda\mu}\mathrm{M}_\mu\mathrm{M}_\lambda) = 0$$

and, by applying Burnside's theorem:

(6) $$h^{\lambda\mu}\mathrm{M}_\mu\mathrm{M}_\lambda = \lambda \,.\, 1.$$

Consequently:

(7) $$\mathcal{H}\mathrm{P}_{nm} = \lambda\mathrm{P}_{nm}, \qquad \text{Q.E.D.}$$

9,1. Theorem II.
If to any eigenvalue of $\mathcal{H}$ belong a finite number of linearly independent eigenfunctions only, then any eigenfunction of $\mathcal{H}$ will be a linear combination of a finite number of matrixelements of irreducible representations.
Proof.
Let $f(G)$ be an eigenfunction. We define as transformed function $\mathcal{T}_{S'}f$ the function with the property.

(1) $$\mathcal{T}_{S'}f(S' \,.\, G) = f(G).$$

For infinitesimal S' this leads to:

(2) $$\mathcal{T}_{S'}f = (1 + \delta\psi^\lambda\mathcal{D}_\lambda)f.$$

Now we have:

(3) $$\mathcal{H}f \doteq \lambda f;$$

(4) $$(1 + \delta\psi^\lambda\mathcal{D}_\lambda)\mathcal{H}f = \lambda(1 + \delta\psi^\lambda\mathcal{D}_\lambda)f;$$

(5) $$\mathcal{H}\{(1 + \delta\psi^\lambda\mathcal{D}_\lambda)f\} = \lambda(1 + \delta\psi^\lambda\mathcal{D}_\lambda)f.$$

Together with f also $\mathcal{T}_{S'}f$ is an eigenfunction belonging to the same eigenvalue. For since this holds for infinitesimal S' it will hold for any S'. But only a finite number of functions $\mathcal{T}_{S'}f$ will be linearly independent; it will be possible to express any $\mathcal{T}_{S'}f$

as a linear combination of a finite number of mutually unitary-orthogonal, normalized functions, f_n. We will have:

(6) $$\mathcal{T}_{S'}f_n(S'G) = f_n(G) = \sum_m \mathrm{R}_{mn}(S')f_m(S'G),$$

where the $\|\mathrm{R}_{mn}(S')\|$ form a unitary representation. By suitably choosing our f_n's it will be possible to reduce this representation. Then

(7) $$f_n(G) = \sum_m \mathrm{P}_{mn}(S')f_m(S'G),$$

(8) $$f_m(S'G) = \sum_n \overline{\mathrm{P}}_{mn}(S')f_n(G)$$

and for the element unity of $\mathfrak{G}$:

(9) $$f_m(S') = \sum_n \overline{\mathrm{P}}_{mn}(S')f_n(E).$$

As together with $\|\mathrm{P}_{mn}\|$ also $\|\overline{\mathrm{P}}_{mn}\|$ forms a representation, our theorem is proved.

10. Theorem III.
The operator $\mathcal{G} = g^{\lambda\mu}\mathcal{D}_\lambda\mathcal{D}_\mu$ commutes with all $\mathcal{D}_\varrho$.
Proof.

(1) $$\mathcal{G}^* \equiv \mathcal{G} + \varepsilon(\mathcal{D}_\varrho\mathcal{G} - \mathcal{G}\mathcal{D}_\varrho) \sim (1 + \varepsilon\mathcal{D}_\varrho)\mathcal{G}(1 - \varepsilon\mathcal{D}_\varrho) = g^{\lambda\mu}\mathcal{D}_\lambda{}^*\mathcal{D}_\mu{}^*,$$

where

(2) $$\mathcal{D}_\lambda{}^* \sim \mathcal{D}_\lambda + \varepsilon(\mathcal{D}_\varrho\mathcal{D}_\lambda - \mathcal{D}_\lambda\mathcal{D}_\varrho) = (\delta_\lambda^\mu + \varepsilon c_{\varrho\lambda}{}^\mu)\mathcal{D}_\mu = \mathrm{P}_\lambda^\mu\mathcal{D}_\mu$$

say.

(3) $$g^{\lambda\mu}\mathcal{D}_\lambda{}^*\mathcal{D}_\mu{}^* = g^{\lambda\mu *}\mathcal{D}_\lambda\mathcal{D}_\mu$$

with

(4) $$g^{\lambda\mu *} = g^{\varrho\sigma}\mathrm{P}_\varrho^\lambda\,\mathrm{P}_\sigma^\mu.$$

(5) $$g_{\lambda\mu}{}^* = c_{\lambda\varrho}{}^{\sigma *} \,.\, c_{\sigma\mu}{}^{\varrho *},$$

where

(6) $$c_{\lambda\varrho}{}^{\sigma *}\mathcal{D}'_\sigma = \mathcal{D}'_\lambda\mathcal{D}'_\varrho - \mathcal{D}'_\varrho\mathcal{D}'_\lambda$$

with

(7) $$\mathfrak{D}'_\lambda = (\delta^\mu_\lambda - \varepsilon c_{\varrho\lambda}{}^\mu)\mathfrak{D}_\mu = (1 - \varepsilon\mathfrak{D}_\varrho)\mathfrak{D}_\lambda(1 + \varepsilon\mathfrak{D}_\varrho).$$

Accordingly

(8) $$c_{\lambda\varrho}{}^{\sigma *} = c_{\lambda\varrho}{}^\sigma$$

and

(9) $$\mathcal{G}^* = \mathcal{G}. \qquad \text{Q.E.D.}$$

10,1. Theorem IV.
$\mathcal{G}$ is selvadjoint.
Proof.

(1) $$\mathcal{G} = g^{\lambda\mu} d^\varrho_\lambda \frac{\partial}{\partial\varphi^\varrho} d^\sigma_\mu \frac{\partial}{\partial\varphi^\sigma} =$$

$$= g^{\lambda\mu} \frac{1}{\left|\operatorname{Det} \| c^\mu_\lambda \|\right|} \cdot \frac{\partial}{\partial\varphi^\varrho} d^\varrho_\lambda \left|\operatorname{Det} \| c^\mu_\lambda \|\right| d^\sigma_\mu \frac{\partial}{\partial\varphi^\sigma}$$

and the operator on the right may easily be seen to be selvadjoint. In order to prove (1) it is sufficiant to prove:

(2) $$\frac{\partial}{\partial\varphi^\varrho}\left[d^\varrho_\lambda \left|\operatorname{Det} \| c^\mu_\lambda \|\right|\right] = 0$$

and this equation is a consequence of the invariance of the element of volume. If φ^λ and $\varphi^{\lambda *}$ are connected by an infinitesimal transformation:

(3) $$\varphi^{\lambda *} = \varphi^\lambda + \delta\psi^\varrho \, . \, d^\lambda_\varrho,$$

we have on the one hand:

(4) $$\left|\operatorname{Det} \| c^\mu_\lambda(\varphi) \|\right| \Pi d\varphi^\varrho = \left|\operatorname{Det} \| c^\mu_\lambda(\varphi^*) \|\right| \Pi d\varphi^{\varrho *}$$

on the other hand:

(5) $$\left|\operatorname{Det} \| c^\mu_\lambda(\varphi^*) \|\right| = \left|\operatorname{Det} \| c^\mu_\lambda(\varphi) \|\right| + \delta\psi^\varrho d^\sigma_\varrho \frac{\partial}{\partial\varphi^\sigma} \left|\operatorname{Det} \| c^\mu_\lambda(\varphi) \|\right|.$$

(6) $$\Pi d\varphi^{\varrho *} = \operatorname{Det} \| \delta^\mu_\lambda + \frac{\partial}{\partial\varphi^\lambda}(d^\mu_\varrho)\,\delta\psi^\varrho \| \; \Pi d\varphi^\varrho =$$

$$= \left[1 + \delta\psi^\varrho \frac{\partial}{\partial\varphi^\lambda}(d^\lambda_\varrho)\right] \Pi d\varphi^\varrho \, .$$

Consequently:

(7) $$d^\sigma_\varrho \frac{\partial}{\partial\varphi^\sigma}\left|\operatorname{Det} \| c^\mu_\lambda(\varphi) \|\right| + \left|\operatorname{Det} \| c^\mu_\lambda(\varphi) \|\right| \frac{\partial}{\partial\varphi^\sigma}(d^\sigma_\varrho) =$$

$$= \frac{\partial}{\partial\varphi^\sigma}\left[d^\sigma_\varrho \left|\operatorname{Det} \| c^\mu_\lambda(\varphi) \|\right|\right] = 0.$$

11. Matrixelements and eigenfunctions.
From theorem IV together with the topological properties of the group it follows:
the eigenfunctions of $\mathcal{G}$ form a complete orthogonal set
to one eigenvalue there belong only a finite number of eigenfunctions
and consequently:
the eigenfunctions of $\mathcal{G}$ are identical with the matrixelements of the irreducible representations of $\mathcal{G}$ and they form a complete orthogonal set.

12. Transformation of more general manifolds.
The investigations of the preceding sections were related to transformations of group space into itself. Let us now consider a realization of $\mathfrak{G}$ by L-transformations of a closed, simply connected continuum $\mathfrak{C}$ into itself. In this case the operator $g^{\lambda\mu}\mathcal{U}_\lambda\mathcal{U}_\mu$ will commute with all $\mathcal{U}_\varrho$, it will be selv-adjoint, the eigenfunctions will form a complete orthogonal set and to one eigenfunction will only belong a finite number of linearly independent eigenfunctions. Using the method of [9, 1] one can show: If C is a point of $\mathfrak{C}$, SC the point into which it is transformed by S the eigenfunctions of $g^{\lambda\mu}\mathcal{U}_\lambda\mathcal{U}_\mu$ satisfy relations:

(1) $$f_n(C) = \sum_m P_{mn}(S) f_m(SC).$$

The eigenfunctions form a complete orthogonal set of functions which are transformed with irreducible representations of our group.

V.

ROTATION OF MOLECULES.

1. Introduction.

In this chapter we will discuss the motion of real systems, of molecules. It is easy to form a qualitative picture of a molecule. The electrons will perform very swift motions not confined to any definite part of our system, the nuclei will swing about their positions of equilibrium and the whole system will be in a (relatively) slow rotation.

In building up the mathematical treatment, one will let oneself lead by this picture of the molecule. First one will keep the nuclei fixed in space and consider the motion of the electrons in the stationary field of the nuclei. One will find that for a certain set of values of the relative distances of the nuclei, the energy has a minimum. This part of the problem may be called chemical. Little has been done in calculating the electronic states. The papers on chemical binding (Heitler-London, Heitler, London, Born, Heitler-Rumer) confine themselves to the investigation of a first approximation for the normal state; it is possible in this way to arrive at a qualitative understanding of many important chemical facts. A more accurate determination of the energy levels and eigenfunctions, however, would — even in simple cases — claim very complicated numerical calculations.

Next one will consider the motion of the nuclei about their positions of equilibrium. We will introduce a set of coordinates depending on the relative distances of the nuclei only and solve the Schrödinger-equation in these coordinates; the interaction with the electrons takes the form of a potential energy, binding the nuclei to their positions of equilibrium. The Raman-effect

has given us a powerful experimental method of determining vibrational terms and much is known already about the modes of vibration of a large number of molecules.

The last problem — which is the one in which we are especially interested — concerns the rotation of our system as a whole. We will consider the motion of a system of heavy particles the relative distances between which are by elastic forces bound to certain equilibrium distances (A), while there are a number of light particles — electrons — the potential energy of which depends on the distances to the equilibrium positions of the nuclei (B).

For a rigorous proof of the legitimacy of this treatment we refer to a paper by Born and Oppenheimer, who showed that it may be regarded as a development in powers of $(m/\mathrm{M})^{\frac{1}{4}}$ (m electronic, M nuclear mass). Our formulation of the rotation problem is correct up to the fourth order. No splitting up of energy levels will occur if we take into account higher powers.

2. General properties of angular momentum.

The angular momentum of a number of particles is defined by:

$$\mathcal{L}_1 = \sum_i \left(y_i \frac{h}{i} \frac{\partial}{\partial z_i} - z_i \frac{h}{i} \frac{\partial}{\partial y_i} \right) \tag{1}$$

and so on.

We have:

$$\mathcal{L}_1 \mathcal{L}_2 - \mathcal{L}_2 \mathcal{L}_1 = ih \mathcal{L}_3 \tag{2}$$

and so on

and for any vectorial function of the coordinates and the p's:

$$\mathcal{L}_1 \mathcal{V}_2 - \mathcal{V}_2 \mathcal{L}_1 = ih \mathcal{V}_3 \tag{3}$$

and so on.

The relations (2) and (3) will be invariant under a transformation of coordinates.

$-\varepsilon(i/h)\, \mathcal{L}_k f(x_i, y_i, z_i)$ is the change of f when an infinitesimal rotation ε about the k-axis is carried out. This geometrical interpretation is often useful if we want to determine the angular momentum in arbitrary coordinates. (The equations (2) are an example of [IV 5 (4)]). If, for instance, we describe a system of

particles by Eulerian angles and a set of parameters depending on the relative distances, then the operators $\mathcal{P}_i$ of [II 8] will correspond to a rotation of all particles simultaneously and therefore be equal to the total angular momentum.

2,1. Electronic spin.

In Pauli's theory of electronic spin a state is not described by one wave function, but by a set of two wavefunctions, a hyperfunction we may call it. A state described by $\begin{cases}\psi_1\\ \psi_2\end{cases}$ in one system of coordinates not described by these two functions expressed in terms of the new variables, $\begin{cases}\psi_1^*\\ \psi_2^*\end{cases}$, $(\psi_i^*(x^*)=\psi_i(x))$ but by $\begin{cases}\psi_1'\\ \psi_2'\end{cases}$, with

$$\begin{aligned}\psi_1' &= S_{11}\psi_1^* + S_{12}\psi_2^*\\ \psi_2' &= S_{21}\psi_1^* + S_{22}\psi_2^*\end{aligned} \tag{1}$$

where $\| S_{ik} \|$ is the two-valued representation discussed in [III 2,2]. The change of a hyperfunction when an infinitesimal rotation is carried out is given by an operator $-\varepsilon\frac{i}{h}\mathcal{J}_i$;

$$\mathcal{J}_i \cdot \begin{cases}\psi_1\\ \psi_2\end{cases} = \begin{cases}\mathcal{L}_i\psi_1 + hM_i(\frac{1}{2})_{11}\psi_1 + hM_i(\frac{1}{2})_{12}\psi_2\\ \mathcal{L}_i\psi_2 + hM_i(\frac{1}{2})_{21}\psi_1 + hM_i(\frac{1}{2})_{22}\psi_2\end{cases} \tag{2}$$

$$\mathcal{J}_i = \mathcal{L}_i + \mathcal{S}_i. \tag{3}$$

The $\mathcal{J}_i$'s satisfy the ordinary relations for the components of angular momentum and so do the $\mathcal{S}_i$. The operators $\mathcal{S}_i$ correspond to the components of the spin momentum. It is easily seen that the eigenvalues of any of the $\mathcal{S}_i$'s are $+\frac{1}{2}h$ and $-\frac{1}{2}h$. We have for instance:

$$\mathcal{S}_3\begin{cases}\psi\\ 0\end{cases} = \tfrac{1}{2}\begin{cases}\psi\\ 0\end{cases};\quad \mathcal{S}_3\begin{cases}0\\ \psi\end{cases} = -\tfrac{1}{2}\begin{cases}0\\ \psi\end{cases}. \tag{4}$$

The transition of wave mechanics to matrix mechanics may be carried out in the same way as in the ordinary Schrödinger theory. Only we have now to develop in terms of a complete orthogonal set of hyperfunctions. We may first use the combinations:

$$\Psi_{n+} = \begin{cases}\psi_n\\ 0\end{cases},\quad \Psi_{n-} = \begin{cases}0\\ \psi_n\end{cases} \tag{5}$$

where the ψ_n form a complete orthogonal set; $\mathcal{S}_i$ will then be represented by $hM_i(\frac{1}{2})$. Next one can introduce linear combinations of these functions such that H becomes a diagonal matrix.

3. Rotation and electronic motion.

We will first discuss problem *B*, assuming that the motion of the system of nuclei may be described by the quantum mechanics of the rigid body. To save writing we will confine ourselves to the case of one electron. Let X, Y, Z be the coordinates of the electron in the ***f***-system, *x*, *y*, *z* in the ***k***-system. The Hamiltonian for the rigid body + the electron is then (we neglect the spin):

$$\frac{1}{2}\left[\frac{Q_1^2}{A_1}+\frac{Q_2^2}{A_2}+\frac{Q_3^2}{A_3}\right]+\frac{1}{2m}(p_X^2+p_Y^2+p_Z^2)+V(x,y,z), \tag{1}$$

(we will no longer distinguish operators by a special type). If we introduce the relative coordinates *x*, *y*, *z* instead of X, Y, Z, we have:

$$p_X^2+p_Y^2+p_Z^2 = p_x^2+p_y^2+p_z^2. \tag{2}$$

In order to calculate the expressions for Q_i in the new variables we observe: $(Q_i)_{x\text{ const.}}\,\psi$ gives the change of ψ when the rigid body is rotated but the electronic coordinates stay the same; $(Q_i)_{x\text{ const.}}\,\psi$ gives the change of ψ when the body is rotated together with the electron, therefore:

$$(Q_i)_{x\text{ const.}} = (Q_i)_{x\text{ const.}} - L_i \tag{3}$$

for $L_i\psi$ gives the change of ψ when only the electron is rotated.

Thus our Hamiltonian becomes:

$$\tfrac{1}{2}\sum_i\frac{1}{A_i}(Q_i-L_i)^2+\frac{1}{2m}(p_x^2+p_y^2+p_z^2)+V(x,y,z). \tag{4}$$

The equation $H\psi = E\psi$ may now approximately be solved as follows: First we solve

$$\left[\frac{1}{2m}(p_x^2+p_y^2+p_z^2)+V(x,y,z)\right]\varphi = E_1\varphi; \tag{5}$$

as $m >> A_i$ this will determine the main part of the energy. If E_1 is a non-degenerate eigenvalue we put $\psi = f \,.\, \varphi$, where f satisfies:

$$(6) \qquad \tfrac{1}{2}\sum_i \frac{1}{A_i}(Q_i^2 - 2Q_i\overline{L_i} + \overline{L_i^2})f = E_2 f;$$

here $\overline{L_i}$ is the mean value of L_i:

$$(7) \qquad \overline{L_i} = \int \bar{\varphi} L_i \varphi.$$

The terms with $\overline{L_i^2}$ give only a constant contribution to the rotational levels. The interesting interaction term is $-\sum Q_i\overline{L_i}/A_i$. For the equations of motion this gives:

$$(8) \qquad \dot{Q}_1 = \tfrac{1}{2}(Q_2Q_3 + Q_3Q_2)\left(\frac{1}{A_3} - \frac{1}{A_2}\right) + \frac{Q_3\overline{L_2}}{A_2} - \frac{Q_2\overline{L_3}}{A_3}.$$

The solution of the matrix problem corresponding to (6) may be carried out in the same way as in the case $\overline{L_i} = 0$: We substitute for Q_i the S-representation and arrive at a $(2j+1)$ dimensional H-matrix. A division into $\boldsymbol{O}$ and $\boldsymbol{E}$ terms is now impossible, the distinction between $+$ and $-$ will still exist.

If E_1 is p-fold degenerate we find for our rotational Hamiltonian:

$$(9) \qquad \tfrac{1}{2}\sum_i \frac{1}{A_i}(Q_i^2 - 2Q_iL_i + L_i^2);$$

L_i will now be a p-dimensional matrix corresponding to the p electronic states that are degenerate with each other. We have now to bring a $p(2j+1)$ dimensional matrix into diagonal form.

A degeneracy is only to be expected if the nuclear field of force has a certain symmetry viz. if the group of symmetry of this field possesses more dimensional irreducible representations.

As to the mean values $\overline{L_i}$ in case of non-degeneracy we remark: If the nuclear field has rotational symmetry about an axis the angular momentum in this direction is an integral and may take all positive and negative integer values. Further it is a general theorem: If the field of force is invariant under an inversion with respect to a plane through a certain axis and if there is no rotational symmetry about this axis, then the mean value of the

angular momentum in direction of this axis is zero. For in this case the electronic wave functions may be divided in $+$ and $-$ functions; the $+$ functions are invariant under the inversion, the $-$ functions change their sign. If we introduce polar coordinates, ϑ, φ, r, where φ is counted from the symmetry plane the $+$ functions will be of the form $\sum a_k \cos k\varphi$ the $-$ functions of the form $\sum b_k \sin k\varphi$. But

$$(10) \qquad \int_0^{2\pi} \sin l\varphi \,.\, \frac{\partial}{\partial\varphi}\sin k\varphi \,.\, d\varphi = 0, \qquad \int_0^{2\pi} \cos l\varphi \,.\, \frac{\partial}{\partial\varphi}\cos k\varphi \,.\, d\varphi = 0:$$

the mean value of the angular momentum in direction of the axis is zero. In other cases a special investigation is necessary.

3,1. Rotation and electronic spin.

If we take into account the electronic spin our Hamiltonian will be given by:

$$(1) \qquad \tfrac{1}{2}\sum \frac{1}{A_i}Q_i^2 + \frac{1}{2m}(p_X^2 + p_Y^2 + p_Z^2) + V(x, y, z) + F$$

where F represents the interaction between spin and orbit This interaction will depend on x, p_X, and the components of the spin momentum in the f-system. The transformation $X \rightarrow x$ will now lead to:

$$(2) \qquad \tfrac{1}{2}\sum \frac{1}{A_i}(Q_i - J_i)^2 + \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + V(x, y, z) + F,$$

where F will no longer depend on the Eulerian angles. This equation is proved in the same way as [3(4)]. If there are more electrons we will arrive at an analogous expression; J_i must then be replaced by $\sum J_i$, the resultant angular momentum of the electrons. As $\sum Q_i^2 = j(j+1)h^2$ is the square modul of the total angular momentum, j has to be an integer if there is an even number of electrons, half an odd integer if the number of electrons is odd.

For an approximate solution of (2) we have to distinguish three cases:

A. The interaction energy between spin and orbit is large compared with the rotational energy.

In this case we will first solve the equation.

$$(3) \qquad \left[\frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + V(x, y, z) + F\right]\varphi = E_1\varphi$$

and the Hamiltonian for the rotations will become:

$$(4) \qquad \tfrac{1}{2}\sum \frac{1}{A_i}(Q_i^2 - 2\overline{J_i}Q_i + \overline{J_i^2}).$$

(If the electronic state is p-fold degenerate we must replace the mean value $\overline{J_i}$ by a p dimensional matrix).

B. The interaction between spin and orbit is of the same order of magnitude as the rotational energy.

In this case we will first solve:

$$(5) \qquad \left[\frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + V(x, y, z)\right]\varphi = E_1\varphi$$

and then the problem with the Hamiltonian

$$(6) \qquad \tfrac{1}{2}\sum \frac{1}{A_i}(Q_i^2 - 2\overline{L_i}Q_i + \overline{L_i^2} + S_i^2 - 2S_iQ_i - 2S_i\overline{L_i}) + \overline{F}$$

$\overline{F}$ will (if the electronic state without spin is non-degenerate) be 2 dimensional and the H-matrices will be $2(2j+1)$ dimensional. (If there are r electrons they will be $2^r(2j+1)$ dimensional.)

C. The interaction between spin and orbit is small compared with the rotational energy.

This will never occur for electrons. But for the nuclear spin this condition will always be fulfilled. Our rotational Hamiltonian will be:

$$(7) \qquad \tfrac{1}{2}\sum \frac{1}{A_i}\left[(Q_i - S_i)^2 - 2\overline{L_i}(Q_i - S_i) + \overline{L_i^2}\right].$$

Now $Q_i - S_i$ satisfies just the same relations as Q_i. We may write:

$$(8) \qquad Q_i^* = Q_i - S_i$$

and set down the S-representation for Q_i^*. $\sum Q_i^{*2} = j(j+1)h$ is

an integral of the equations of motion. As Q_i^* does not involve the spin momentum, j will in this case be an integer. The problem is just as if there were no spin at all. In a higher approximation the spin may give rise to hyperfinestructure.

4. Rotation and vibrations.

We have now to investigate the motion of a system of heavy particles, bound by elastic forces to a position of equilibrium. The problem is whether the rotation of such a system will be described by the quantum mechanics of the rigid body, whether there will be certain interaction terms, or whether there will be no connection whatever between this theory and the motion of our system. Even if we assume that the forces are strong, so that the amplitudes of the vibrations will be small, the answer is not quite obvious. There is a fundamental difference with the corresponding classical problem: if the forces are increased also the frequency will be increased and therewith the energy of the lowest possible state, $\frac{1}{2}h\omega$. If the potential energy of an oscillator is given by $\frac{1}{2}ku^2$ (u deviation from normal position) then the frequency will be given by $\sqrt{k/m}$ and the energy of the lowest state by $\frac{1}{2}h\sqrt{k/m}$. The amplitude will be $\sim k^{-\frac{1}{4}}$ the maximum velocity however $\sim k^{\frac{1}{4}}$.

As I have not yet been able to find a satisfactory treatment of the general problem, I will in the following confine myself to the discussion of a simplified problem, which, I hope, will show some of the essential factures of the general case.

4,1. Discussion of simplified model.

We will discuss the motion of a "rigid body" to a certain point of which a heavy particle is bound by forces such that the amplitude of the vibrations of this particle may be regarded a small. We will further assume that the body is so heavy that the difference between the centre of gravity of the body and that of the body + particle may be neglected.

We will start in the same way as in the preceding section; the Hamiltonian will again become:

$$(1)\qquad \tfrac{1}{2}\sum \frac{1}{A_i}(Q_i - L_i)^2 + \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + V(x, y, z.)$$

Next we will write $x = x_0 + \xi$, $y = y_0 + \eta$, $z = z_0 + \zeta$ where x_0, y_0, z_0 are the coordinates of the equilibrium position in the k-system. We have:

$$(2)\qquad L_1 = y_0 p_\zeta - z_0 p_\eta + \eta p_\zeta - \zeta p_\eta.$$

The last two terms are of the order of magnitude h (for low vibrational quantum numbers) and they will stay of the same order when the frequency of the vibration tends to infinity. The first two terms, however, will be large compared with Q_i and they make it impossible at once to write down an approximate solution of (1). We will remove them from the wave equation by a substitution of the form:

$$(3)\qquad \psi = \exp\left\{\frac{i}{h}(f_1\xi + f_2\eta + f_3\zeta)\right\}\psi'$$

where f_i does not depend on ξ, p_ξ.
We will introduce the following notation: $\widetilde{Q}$ is the row Q_1, Q_2, Q_3;

$$Q \text{ is the column } \begin{cases} Q_1 \\ Q_2 \\ Q_3 \end{cases}$$

$\widetilde{p}$ is the row p_ξ, p_η, p_ζ; p the corresponding column.
Further we write:

$$(4)\qquad L = N(x)\,p = N_0 p + N(\xi)p$$

with

$$(5,\,6)\qquad N(x) = \begin{Vmatrix} 0 & -z & y \\ z & 0 & -x \\ -y & x & 0 \end{Vmatrix};\quad N_0 = \begin{Vmatrix} 0 & -z_0 & y_0 \\ z_0 & 0 & -x_0 \\ -y_0 & x_0 & 0 \end{Vmatrix};$$

$$(7)\qquad N(\xi) = \begin{Vmatrix} 0 & -\zeta & \eta \\ \zeta & 0 & -\xi \\ -\eta & \xi & 0 \end{Vmatrix}.$$

A is the matrix of inertia, A^{-1} its reciprocal. Our Hamiltonian becomes:

$$\tfrac{1}{2}[\widetilde{Q}A^{-1}Q - \widetilde{p}\widetilde{N}_0A^{-1}Q - QA^{-1}N_0p + \widetilde{p}\widetilde{N}_0A^{-1}N_0p + \frac{1}{m}\widetilde{p}Ep +$$

$$(8)\qquad +2V - \widetilde{p}\widetilde{N}(\xi)A^{-1}Q - \widetilde{Q}A^{-1}N(\xi)p + \widetilde{p}\widetilde{N}(\xi)A^{-1}N_0p +$$
$$+\widetilde{p}\widetilde{N}_0A^{-1}N(\xi)p + \widetilde{p}\widetilde{N}(\xi)A^{-1}N(\xi)p].$$

By means of (3) p is transformed into $p + f$. If we first leave out the terms with $N(\xi)$ we get:

$$\tfrac{1}{2}[\widetilde{Q}A^{-1}Q - \widetilde{p}\widetilde{N}_0A^{-1}Q - \widetilde{f}\widetilde{N}_0A^{-1}Q - \widetilde{Q}A^{-1}N_0p - \widetilde{Q}A^{-1}N_0f +$$

$$(9)\qquad +\widetilde{f}\widetilde{N}_0A^{-1}N_0f + \widetilde{p}\widetilde{N}_0A^{-1}N_0f + \widetilde{f}\widetilde{N}_0A^{-1}N_0p + \widetilde{p}\widetilde{N}_0A^{-1}N_0p +$$
$$+\frac{1}{m}\widetilde{p}Ep + \frac{1}{m}\widetilde{f}Ep + \frac{1}{m}\widetilde{p}Ef + \frac{1}{m}\widetilde{f}Ef + 2V].$$

If we now choose f such that

$$(10)\qquad (\widetilde{N}_0A^{-1}N_0 + \frac{1}{m}E)f = \widetilde{N}_0A^{-1}Q,$$

the terms $-\widetilde{p}\widetilde{N}_0A^{-1}Q$ and automatically also the terms $-\widetilde{Q}A^{-1}N_0p$ will be removed. We then have:

$$(11)\qquad f = \left(\frac{1}{m}E + \widetilde{N}_0A^{-1}N_0\right)^{-1}.\,\widetilde{N}_0A^{-1}Q = m\widetilde{N}_0(A + mN_0\widetilde{N}_0)^{-1}.\,Q;$$

$$(12)\qquad \widetilde{f} = \widetilde{Q}(A + mN_0\widetilde{N}_0)^{-1}.\,mN_0.$$

Now $mN_0\widetilde{N}_0$ is the matrix:

$$(13)\qquad mN_0\widetilde{N}_0 = \begin{Vmatrix} m(y^2+z^2) & -mxy & -mxz \\ -mxy & m(x^2+z^2) & -myz \\ -mxz & -myz & m(y^2+x^2) \end{Vmatrix}.$$

$A + mN_0\widetilde{N}_0$ will accordingly be the matrix of inertia of the rigid body together with the heavy particle in its equilibrium position. Our Hamiltonian becomes (we still omit the terms with $N(\xi)$):

$$\tfrac{1}{2}[\widetilde{Q}\{A^{-1} - (A+mN_0\widetilde{N}_0)^{-1}.mN_0\widetilde{N}_0A^{-1} - A^{-1}.mN_0\widetilde{N}_0(A+mN_0\widetilde{N}_0)^{-1} +$$
$$+(A+mN_0\widetilde{N}_0)^{-1}.mN_0\widetilde{N}_0A^{-1}.mN_0\widetilde{N}_0(A+mN_0\widetilde{N}_0)^{-1} +$$
$$(14)\qquad +(A+mN_0\widetilde{N}_0)^{-1}.mN_0\widetilde{N}_0(A+mN_0\widetilde{N}_0)^{-1}\}Q +$$
$$+\widetilde{p}(\widetilde{N}_0A^{-1}N_0 + \frac{1}{m}E)p] + V =$$

$$= \tfrac{1}{2}[\widetilde{Q}(A + mN_0\widetilde{N}_0)^{-1}\{(A + mN_0\widetilde{N}_0)A^{-1}(A + mN_0\widetilde{N}_0) -$$
$$- mN_0\widetilde{N}_0A^{-1} \cdot (A + mN_0\widetilde{N}_0) - (A + mN_0\widetilde{N}_0)A^{-1} \cdot mN_0\widetilde{N}_0 +$$
(15) $$+ mN_0\widetilde{N}_0A^{-1} \cdot mN_0\widetilde{N}_0 + mN_0\widetilde{N}_0\{(A + mN_0\widetilde{N}_0)^{-1} \cdot Q +$$
$$+ \widetilde{p}(\widetilde{N}_0A^{-1} \cdot N_0 + \frac{1}{m}E)p] + V =$$

(16) $$= \tfrac{1}{2}[\widetilde{Q}(A + mN_0\widetilde{N}_0)^{-1}Q + \widetilde{p}(\widetilde{N}_0A^{-1}N_0 + \frac{1}{m}E)p] + V$$

Next we have to calculate the correction terms involving $N(\xi)$. We will only consider the terms containing both p (or $\widetilde{p}$) and $N(\xi)$ (or $\widetilde{N}(\xi)$).
They are:

$$\tfrac{1}{2}[-\widetilde{p}\,\widetilde{N}(\xi)A^{-1} \cdot Q + \widetilde{p}\,\widetilde{N}(\xi)A^{-1} \cdot mN_0\widetilde{N}_0(A + mN_0\widetilde{N}_0)^{-1} \cdot Q +$$
$$+ \widetilde{p}\,\widetilde{N}_0A^{-1} \cdot N(\xi)m\widetilde{N}_0(A + mN_0\widetilde{N}_0)^{-1} \cdot Q - \widetilde{Q}A^{-1} \cdot N(\xi)p +$$
(17) $$+ \widetilde{Q}(A + mN_0\widetilde{N}_0)^{-1} \cdot mN_0\widetilde{N}_0A^{-1} \cdot N(\xi)p +$$
$$+ \widetilde{Q}(A + mN_0\widetilde{N}_0)^{-1} \cdot mN_0\widetilde{N}(\xi)A^{-1} \cdot N_0p +$$
$$+ \widetilde{p}\,\widetilde{N}(\xi)A^{-1} \cdot N_0p + \widetilde{p}\,\widetilde{N}_0A^{-1} \cdot N(\xi)p + \widetilde{p}\,\widetilde{N}(\xi)A^{-1} \cdot N(\xi)p].$$

Our Hamiltonian will now be of the form:

$$T(\widetilde{p}, p, \xi) + V(\xi) + \tfrac{1}{2}[\widetilde{Q}(A + mN_0\widetilde{N}_0)^{-1} \cdot Q -$$
(18) $$- \widetilde{F}(A + mN_0\widetilde{N}_0)^{-1} \cdot Q - \widetilde{Q}(A + mN_0\widetilde{N}_0)^{-1} \cdot F].$$

The wave equation may now again be solved approximately, by first solving:

(19) $$\{T(\widetilde{p}, p, \xi) + V(\xi)\}\varphi = E\varphi$$

and then the rotation problem with the Hamiltonian:

(20) $$\tfrac{1}{2}[\widetilde{Q}(A + mN_0\widetilde{N}_0)^{-1} \cdot Q - \overline{F}(A + mN_0\widetilde{N}_0)^{-1} \cdot Q -$$
$$- \widetilde{Q}(A + mN_0\widetilde{N}_0)^{-1} \cdot \overline{F}].$$

The interaction, F, is given by:

(21) $$F = N(\xi)p - m\,N_0\widetilde{N}(\xi)A^{-1} \cdot N_0p.$$

This expression will be of the order h and remain of the same order when the frequency is increased; for our purpose it is not necessary nearer to investigate its mean value.

Our conclusion is: the motion of our system may approximately be divided into vibration and rotation. The Hamiltonian for the rotations is that of the rigid body together with the heavy particle + certain interaction terms between rotation and vibration of the order of magnitude h. For high rotational quantum numbers the influence of these interaction terms will disappear.

5. Rotation and vibrations; general case.

The result of the preceding section suggests: the motion of a system of particles may be divided into rotation and vibrations. The Hamiltonian for the rotation is that of a rigid body with a tensor of inertia calculated for the equilibrium positions of the particles + interaction terms of the order h:

(1) $$H = \tfrac{1}{2}\Sigma \frac{1}{A_i}(Q_i^2 - 2\overline{F}_iQ_i).$$

Indeed, the preceding section may be regarded more or less as a proof by complete induction of this result. For high rotational quantum numbers the influence of the interaction terms will vanish; in the limit of classical mechanics we will therefore obtain the ordinary equations for the rigid body.

But here the really physical problems first start. What will $\overline{F}$ be for a real molecule? In which way does it depend on the properties of symmetry of a molecule? Under which general conditions will it vanish? What do we learn from the application of our formulae to the analysis of rotation bands?

All these questions remain unanswered. Yet I hope that this chapter, however incomplete it may be, will show the usefulness of the symbolic methods, that form the main subject of this book.

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V.

M. BORN und J. R. OPPENHEIMER; Ann. d. Phys. **84**, 457, 1927.

[3, 1 (2)] given by WANG; loc. cit. II.

CONTENTS.

C 3

H.B.G. Casimir

STELLINGEN.

I.

De asymptotiese uitdrukkingen voor cylinderfuncties, die gewoonlik (b.v. in Courant-Hilbert) met behulp van de zadelpuntmetode worden afgeleid, kunnen ook uit de differentiaalvergelijking worden verkregen.

Courant-Hilbert. Methoden der mathematischen Physik. Kap. VII.

II.

Dat er op een bol geen stel kontinue functies aan te geven is, die zich transformeren volgens een tweeduidige irreducibele representatie van de draaiingsgroep, kan worden afgeleid uit het feit, dat de eigenwaarden der infinitesimale elementen van deze representaties alle ongelijk nul zijn.

Deze stelling kan worden uitgebreid op algemene kontinue groepen.

III.

Uit de differentiaalvergelijking voor de matrixelementen der irreducibele representaties van een kontinue groep, kan een differentiaalvergelijking voor de karakters worden afgeleid.

IV.

Het verdient aanbeveling de notatie bgtg te vervangen door arctg.

V.

Wil men een "round the corner straight" als geldig spel erkennen, dan moet men er dezelfde waarde aan toekennen als aan een gewone straight. De kritiek hierop door R. F. Foster uitgeoefend houdt geen steek.

Enc. Britt. 14de druk; 18, ~~589.~~ 126 127.

VI.

De "shimmy" van een auto berust op een tolwerking der wielen.

VII.

De fotoelektriese absorptie van zeer harde gammastralen is ook voor zware atomen evenredig met de golflengte.

VIII.

Bij de discussie van de al of niet geldigheid van de formule van Klein-Nishina en bij het toepassen ervan, dient men rekening te houden: *a.* met het fotoeffekt; *b.* met de invloed van de binding op het Comptoneffekt.

IX.

De opmerkingen van A. Tschermak tonen geenszins de onjuistheid of onvolledigheid der fysiese driekleurenteorie aan.

Naturw. 18, 589, 1930.

X.

Een verschil tussen "ortho-" en "para"stikstof zou misschien vast te stellen zijn door een onderzoek van de intensiteitswisseling in het bandenspectrum na bewaring bij lage temperaturen.

Een verschil in de soortelike warmte is wel nauweliks meetbaar.

XI.

Het is wenselik de elasticiteitskonstanten en uitzettingskoefficienten van metalen bij lage temperaturen te meten. Dergelike metingen zouden kunnen bijdragen tot het verkrijgen van een inzicht, welke eigenschappen het zijn, die een suprageleidend metaal van een niet suprageleidend metaal onderscheiden.

XII.

Vooral Bohr heeft er op gewezen, dat men er op voorbereid moet zijn, dat bij kernprocessen de wet van behoud van arbeidsvermogen niet meer geldt. Dit voert met zich mee dat men, ook in de astrofysika, de relatie $M = E/c^2$ niet meer als zeker mag beschouwen.