Quantisation as a Problem of
Proper Values (Part II)

§ 1. The Hamiltonian Analogy between Mechanics and Optics

BEFORE we go on to consider the problem of proper values for further special systems, let us throw more light on the *general* correspondence which exists between the Hamilton-Jacobi differential equation of a mechanical problem and the "allied" *wave equation*, *i.e.* equation (5) of Part I. in the case of the Kepler problem. So far we have only briefly described this correspondence on its external analytical side by the transformation (2), which is in itself unintelligible, and by the equally incomprehensible transition from the *equating to zero* of a certain expression to the postulation that the *space integral* of the said expression shall be *stationary*.[1]

The *inner* connection between Hamilton's theory and the process of wave propagation is anything but a new idea. It was not only well known to Hamilton, but it also served him as the starting-point for his theory of mechanics, which grew [2] out of his *Optics of Non-homogeneous Media*. Hamilton's variation principle can be shown to correspond to Fermat's *Principle* for a wave propagation in configuration space (*q*-space), and the Hamilton-Jacobi equation expresses Huygens' *Principle* for this wave propagation. Unfortunately this powerful and momentous conception of Hamilton is deprived, in most modern reproductions, of its beautiful raiment as a superfluous accessory, in favour of a more colourless representation of the analytical correspondence.[3]

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[1] This procedure will *not be pursued further* in the present paper. It was only intended to give a provisional, quick survey of the external connection between the wave equation and the Hamilton-Jacobi equation. ψ is not actually the action function of a definite motion in the relation stated in (2) of Part I. On the other hand the connection between the wave equation and the variation problem is of course very real; the integrand of the stationary integral is the Lagrange function for the wave process.

[2] Cf. *e.g.* E. T. Whittaker's *Anal. Dynamics*, chap. xi.

[3] Felix Klein has since 1891 repeatedly developed the theory of Jacobi from quasi-optical considerations in non-Euclidean higher space in his lectures on mechanics. Cf. F. Klein, *Jahresber. d. Deutsch. Math. Ver.* 1, 1891, and *Zeits. f. Math. u. Phys.* 46,

Let us consider the general problem of conservative systems in classical mechanics. The Hamilton-Jacobi equation runs

(1)
$$\frac{\partial W}{\partial t} + T\left(q_k, \frac{\partial W}{\partial q_k}\right) + V(q_k) = 0.$$

W is the action function, *i.e.* the time integral of the Lagrange function $T - V$ along a path of the system as a function of the end points and the time. q_k is a representative position co-ordinate ; T is the kinetic energy as function of the q's and momenta, being a quadratic form of the latter, for which, as prescribed, the partial derivatives of W with respect to the q's are written. V is the potential energy. To solve the equation put

(2) $W = - Et + S(q_k),$

and obtain

(1')
$$2T\left(q_k, \frac{\partial W}{\partial q_k}\right) = 2(E - V).$$

E is an arbitrary integration constant and signifies, as is known, the energy of the system. Contrary to the usual practice, we have let the function W remain itself in (1'), instead of introducing the time-free function of the co-ordinates, S. That is a mere superficiality.

Equation (1') can now be very simply expressed if we make use of the method of Heinrich Hertz. It becomes, like all geometrical assertions in configuration space (space of the variables q_k), especially simple and clear if we introduce into this space a non-Euclidean metric by means of the kinetic energy of the system.

Let $\overline{T}$ be the kinetic energy as function of the velocities $\dot{q}_k$, not of the *momenta* as above, and let us put for the line element

(3) $ds^2 = 2\overline{T}(q_k, \dot{q}_k)dt^2.$

The right-hand side now contains dt only externally and represents (since $\dot{q}_k dt = dq_k$) a quadratic form of the dq_k's.

After this stipulation, conceptions such as angle between two line elements, perpendicularity, divergence and curl of a vector, gradient of a scalar, Laplacian operation (= div grad) of a scalar, and others, may be used in the same simple way as in three-dimensional Euclidean space, and we may use in our thinking the Euclidean three-dimensional representation with impunity, except that the analytical expressions for these ideas become a very little more complicated, as the line element (3) must everywhere replace the Euclidean line element. *We stipulate, that in what follows, all geometrical statements in q-space are to be taken in this non-Euclidean sense.*

One of the most important modifications for the calculation is

1901 (*Ges.-Abh.* ii. pp. 601 and 603). In the second note, Klein remarks reproachfully that his discourse at Halle ten years previously, in which he had discussed this correspondence and emphasized the great significance of Hamilton's optical works, had "not obtained the general attention, which he had expected". For this allusion to F. Klein, I am indebted to a friendly communication from Prof. Sommerfeld. See also *Atombau*, 4th ed., p. 803.

that we must distinguish carefully between covariant and contravariant components of a vector or tensor. But this complication is not any greater than that which occurs in the case of an oblique set of Cartesian axes.

The dq_k's are the prototype of a contravariant vector. The coefficients of the form $2\bar{T}$, which depend on the q_k's, are therefore of a covariant character and form the covariant fundamental tensor. $2T$ is the contravariant form belonging to $2\bar{T}$, because the momenta are known to form the covariant vector belonging to the speed vector $\dot{q}_k$, the momentum being the velocity vector in covariant form. The left side of (1′) is now simply the contravariant fundamental form, in which the $\dfrac{\partial W}{\partial q_k}$'s are brought in as variables. The latter form the components of the vector,—according to its nature covariant,

$$\text{grad } W.$$

(The expressing of the kinetic energy in terms of momenta instead of speeds has then *this* significance, that covariant vector components can only be introduced in a contravariant form if something intelligible, *i.e.* invariant, is to result.)

Equation (1′) is equivalent thus to the simple statement

(1″) $$(\text{grad } W)^2 = 2(E - V),$$

or

(1‴) $$|\text{grad } W| = \sqrt{2(E - V)}.$$

This requirement is easily analysed. Suppose that a function W, of the form (2), has been found, which satisfies it. Then this function can be clearly represented for every definite t, if the family of surfaces $W = \text{const.}$ be described in q-space and to each member a value of W be ascribed.

Now, on the one hand, as will be shown immediately, equation (1‴) gives an exact rule for constructing all the other surfaces of the family and obtaining their W-values from any single member, *if the latter and its W-value is known*. On the other hand, if the sole necessary data for the construction, viz. *one* surface and its W-value be *given quite arbitrarily*, then from the rule, which presents just *two* alternatives, there may be completed one of the functions W fulfilling the given requirement. Provisionally, the time is regarded as constant.—The construction rule therefore *exhausts* the contents of the differential equation; *each* of its solutions can be obtained from a suitably chosen surface and W-value.

Let us consider the construction rule. Let the value W_0 be given in Fig. 1 to an arbitrary surface. In order to find the surface $W_0 + dW_0$, take *either* side of the given surface as the positive one, erect the normal at each point of it and cut off (with due regard to the sign of dW_0) the *step*

(4) $$ds = \frac{dW_0}{\sqrt{2(E - V)}}.$$

The locus of the end points of the steps is the surface $W_0 + dW_0$. Similarly, the family of surfaces may be constructed successively on both sides.
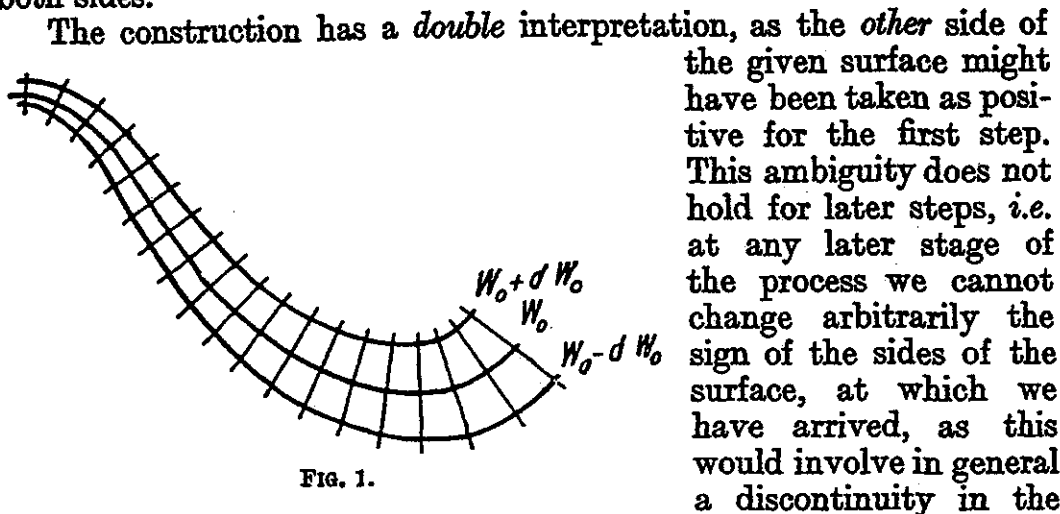
The construction has a *double* interpretation, as the *other* side of the given surface might have been taken as positive for the first step. This ambiguity does not hold for later steps, *i.e.* at any later stage of the process we cannot change arbitrarily the sign of the sides of the surface, at which we have arrived, as this would involve in general a discontinuity in the first differential coefficient of W. Moreover, the two families obtained in the two cases are clearly identical; the W-values merely run in the opposite direction.

FIG. 1.

Let us consider now the very simple dependence on the *time*. For this, (2) shows that at any later (or earlier) instant $t + t'$, the *same* group of surfaces illustrates the W-distribution, though different W-values are associated with the individual members, namely, from each W-value ascribed at time t there must be subtracted Et'. The W-values wander, as it were, from surface to surface according to a definite, simple law, and for positive E in the direction of W increasing. Instead of this, however, we may imagine that the *surfaces* wander in such a way that each of them continually takes the place and exact form of the following one, and always carries its W-value *with* it. The rule for this wandering is given by the fact that the surface W_0 at time $t + dt$ must have reached *that* place, which at t was occupied by the surface $W_0 + Edt$. This will be attained according to (4), if each point of the surface W_0 is allowed to move in the direction of the positive normal through a distance

$$(5) \qquad ds = \frac{Edt}{\sqrt{2(E - V)}}.$$

That is, the surfaces move with a *normal velocity*

$$(6) \qquad u = \frac{ds}{dt} = \frac{E}{\sqrt{2(E - V)}},$$

which, when the constant E is given, is a pure function of position.

Now it is seen that our system of surfaces $W = \text{const.}$ can be conceived as the system of wave surfaces of a progressive but stationary wave motion in q-space, for which the value of the phase velocity at every point in the space is given by (6). For the normal construction

can clearly be replaced by the construction of elementary Huygens waves (with radius (5)), and then of their envelope. The "index of refraction" is proportional to the reciprocal of (6), and is dependent on the position but not on the direction. The q-space is thus optically non-homogeneous but is isotropic. The elementary waves are "spheres", though of course—let me repeat it expressly once more—in the sense of the line-element (3).

The function of action W plays the part of the *phase* of our wave system. The Hamilton-Jacobi equation is the expression of Huygens' principle. If, now, Fermat's principle be formulated thus,

$$(7) \qquad 0 = \delta \int_{P_1}^{P_2} \frac{ds}{u} = \delta \int_{P_1}^{P_2} \frac{ds\sqrt{2(E-V)}}{E} = \delta \int_{t_1}^{t_2} \frac{2T}{E} dt = \frac{1}{E} \delta \int_{t_1}^{t_2} 2T dt,$$

we are led directly to Hamilton's principle in the form given by Maupertuis (where the time integral is to be taken with the usual grain of salt, *i.e.* $T+V=E=$ constant, even during the variation). The "rays", *i.e.* the orthogonal trajectories of the wave surfaces, are therefore the *paths* of the system for the value E of the energy, in agreement with the well-known system of equations

$$(8) \qquad p_k = \frac{\partial W}{\partial q_k},$$

which states, that a set of system paths can be derived from each special function of action, just like a fluid motion from its velocity potential.[1] (The momenta p_k form the covariant velocity vector, which equations (8) assert to be equal to the gradient of the function of action.)

Although in these deliberations on wave surfaces we speak of velocity of propagation and Huygens' principle, we must regard the analogy as one between mechanics and *geometrical* optics, and not physical or *undulatory* optics. For the idea of "rays", which is the essential feature in the mechanical analogy, belongs to *geometrical* optics; it is only clearly defined in the latter. Also Fermat's principle can be applied in geometrical optics without going beyond the idea of index of refraction. And the system of W-surfaces, regarded as wave surfaces, stands in a somewhat looser relationship to mechanical motion, inasmuch as the image point of the mechanical system in no wise moves along the ray with the wave velocity u, but, on the contrary, its velocity (for constant E) is proportional to $\frac{1}{u}$. It is given directly from (3) as

$$(9) \qquad v = \frac{ds}{dt} = \sqrt{2T} = \sqrt{2(E-V)}.$$

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[1] See especially A. Einstein, *Verh. d. D. Physik. Ges.* 19, pp. 77, 82, 1917. The framing of the quantum conditions here is the most akin, out of all the older attempts, to the present one. De Broglie has returned to it.

This non-agreement is obvious. Firstly, according to (8), the system's point velocity is *great* when grad W is great, *i.e.* where the W-surfaces are closely crowded together, *i.e.* where u is small. Secondly, from the definition of W as the time integral of the Lagrange function, W *alters* during the motion (by $(T - V)dt$ in the time dt), and so the image point *cannot* remain continuously in contact with the same W-surface.

And important ideas in wave theory, such as amplitude, wave length, and frequency—or, speaking more generally, the wave *form*—do not enter into the analogy at all, as there exists no mechanical parallel ; even of the wave function itself there is no mention beyond that W has the meaning of the *phase* of the waves (and this is somewhat hazy owing to the wave *form* being undefined).

If we find in the whole parallel merely a satisfactory means of contemplation, then this defect is not disturbing, and we would regard any attempt to supply it as idle trifling, believing the analogy to be precisely with *geometrical*, or at furthest, with a very primitive form of wave optics, and not with the fully developed undulatory optics. That geometrical optics is only a rough approximation for *Light* makes no difference. To *preserve* the analogy on the further development of the optics of q-space on the lines of wave theory, we must take good care not to depart markedly from the limiting case of geometrical optics, *i.e.* must choose [1] the *wave length* sufficiently small, *i.e.* small compared with all the path dimensions. Then the additions do not teach anything new ; the picture is only draped with superfluous ornaments.

So we might think to begin with. But even the first attempt at the development of the analogy to the wave theory leads to such striking results, that a quite different suspicion arises : *we know to-day, in fact, that our classical mechanics fails for very small dimensions of the path and for very great curvatures.* Perhaps this failure is in strict analogy with the failure of geometrical optics, *i.e.* " the optics of infinitely small wave lengths ", that becomes evident as soon as the obstacles or apertures are no longer great compared with the real, finite, wave length. Perhaps our classical mechanics is the *complete* analogy of geometrical optics and as such is wrong and not in agreement with reality ; it fails whenever the radii of curvature and dimensions of the path are no longer great compared with a certain wave length, to which, in q-space, a real meaning is attached. Then it becomes a question of searching [2] for an undulatory mechanics, and the most obvious way is the working out of the Hamiltonian analogy on the lines of undulatory optics.

[1] Cf. for the optical case, A. Sommerfeld and Iris Runge, *Ann. d. Phys.* 35, p. 290, 1911. There (in the working out of an oral remark of P. Debye), it is shown how the equation of *first* order and *second* degree for the *phase* (" Hamiltonian equation ") may be accurately derived from the equation of the *second* order and *first* degree for the *wave function* (" wave equation "), in the limiting case of vanishing wave length.

[2] Cf. A. Einstein, *Berl. Ber.* p. 9 *et seq.*, 1925.

§ 2. " Geometrical " and " Undulatory " Mechanics

We will at first assume that it is fair, in extending the analogy, to imagine the above-mentioned wave system as consisting of *sine* waves. This is the simplest and most obvious case, yet the *arbitrariness*, which arises from the *fundamental significance* of this assumption, must be emphasized. The wave function has thus only to contain the time in the form of a factor, sin (. . .), where the argument is a linear function of W. The coefficient of W must have the dimensions of the reciprocal of action, since W has those of action and the phase of a sine has zero dimensions. We assume that it is quite universal, *i.e.* that it is not only independent of E, but also of the nature of the mechanical system. We may then at once denote it by $\frac{2\pi}{h}$. The time factor then is

$$(10) \qquad \sin\left(\frac{2\pi W}{h} + \text{const.}\right) = \sin\left(-\frac{2\pi Et}{h} + \frac{2\pi S(q_k)}{h} + \text{const.}\right).$$

Hence the *frequency* ν of the waves is given by

$$(11) \qquad\qquad \nu = \frac{E}{h}.$$

Thus we get the frequency of the q-space waves to be proportional to the energy of the system, in a manner which is not markedly artificial.[1] This is only true of course if E is absolute and not, as in classical mechanics, indefinite to the extent of an additive constant. By (6) and (11) the *wave length* is *independent* of this additive constant, being

$$(12) \qquad\qquad \lambda = \frac{u}{\nu} = \frac{h}{\sqrt{2(E-V)}},$$

and we know the term under the root to be double the kinetic energy. Let us make a preliminary rough comparison of this wave length with the dimensions of the orbit of a hydrogen electron as given by classical mechanics, taking care to notice that a " step " in q-space has not the dimensions of length, but length multiplied by the square root of mass, in consequence of (3). λ has similar dimensions. We have therefore to divide λ by the dimension of the orbit, a cm., say, and by the square root of m, the mass of the electron. The quotient is of the order of magnitude of

$$\frac{h}{mva},$$

where v represents for the moment the electron's velocity (cm./sec.). The denominator mva is of the order of the mechanical moment of momentum, and this is at least of the order of 10^{-27} for Kepler orbits, as can be calculated from the values of electronic charge and mass

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[1] In Part I. this appeared merely as an approximate equation, derived from a pure speculation.

independently of all quantum theories. We thus obtain the correct order for the *limit of the approximate region of validity of classical mechanics*, if we identify our constant h with Planck's quantum of action—and this is only a preliminary attempt.

If in (6), E is expressed by means of (11) in terms of ν, then we obtain

(6')
$$u = \frac{h\nu}{\sqrt{2(h\nu - V)}}.$$

The dependence of the wave velocity on the energy thus becomes a particular kind of dependence on the *frequency*, *i.e.* it becomes a *law of dispersion* for the waves. This law is of great interest. We have shown in § 1 that the wandering wave surfaces are only loosely connected with the motion of the system point, since their velocities are not equal and cannot be equal. According to (9), (11), and (6') the system's velocity v has thus also a concrete significance for the wave. We verify at once that

(13)
$$v = \frac{d\nu}{d\left(\dfrac{\nu}{u}\right)},$$

i.e. the velocity of the system point is that of a *group of waves*, included within a small range of frequencies (signal-velocity). We find here again a theorem for the " phase waves " of the electron, which M. de Broglie had derived, with essential reference to the relativity theory, in those fine researches,[1] to which I owe the inspiration for this work. We see that the theorem in question is of wide generality, and does not arise solely from relativity theory, but is valid for every conservative system of ordinary mechanics.

We can utilise this fact to institute a much more innate connection between wave propagation and the movement of the representative point than was possible before. We can attempt to build up a wave group which will have relatively small dimensions in every direction. Such a wave group will then presumably obey the same laws of motion as a single image point of the mechanical system. It will then give, so to speak, an *equivalent* of the image point, so long as we can look on it as being approximately confined to a point, *i.e.* so long as we can neglect any spreading out in comparison with the dimensions of the path of the system. This will only be the case when the path dimensions, and especially the radius of curvature of the path, are very great compared with the wave length. For, in analogy with ordinary optics, it is obvious from what has been said that not only must the dimensions of the wave group not be reduced below the order of magnitude of the wave length, but, on the contrary, the group must extend in all directions over a large number of wave lengths, if it is to be *approximately monochromatic*. This, however, must be postulated, since the wave group must move about as a whole with a definite

[1] L. de Broglie, *Ann. de Physique* (10) 3, p. 22, 1925. (Thèses, Paris, 1924.)

group velocity and correspond to a mechanical system *of definite energy* (cf. equation 11).

So far as I see, such groups of waves can be constructed on exactly the same principle as that used by Debye [1] and von Laue [2] to solve the problem in ordinary optics of giving an exact analytical representation of a cone of rays or of a sheaf of rays. From this there comes a very interesting relation to that part of the Hamilton-Jacobi theory not described in § 1, viz. the well-known derivation of the equations of motion in integrated form, by the differentiation of a complete integral of the Hamilton-Jacobi equation with respect to the constants of integration. As we will see immediately, the system of equations called after Jacobi is equivalent to the statement : the image point of the mechanical system continuously corresponds to *that* point, where a certain continuum of wave trains coalesces in *equal phase*.

In optics, the representation (strictly on the wave theory) of a " sheaf of rays " with a sharply defined finite cross-section, which proceeds to a focus and then diverges again, is thus carried out by Debye. A *continuum* of *plane* wave trains, each of which alone would fill the *whole* space, is superposed. The *continuum* is produced by letting the wave normal vary throughout the given solid angle. The waves then destroy one another almost completely by interference outside a certain double cone ; they represent exactly, on the wave theory, the desired limited sheaf of rays and also the diffraction phenomena, necessarily occasioned by the limitation. We can represent in this manner an *infinitesimal* cone of rays just as well as a finite one, if we allow the wave normal of the group to vary only inside an infinitesimal solid angle. This has been utilised by von Laue in his famous paper on the degrees of freedom of a sheaf of rays.[3] Finally, instead of working with waves, hitherto tacitly accepted as purely monochromatic, we can also allow the *frequency* to vary within an infinitesimal interval, and by a suitable distribution of the amplitudes and phases can confine the disturbance to a region which is relatively small in the longitudinal direction also. So we succeed in representing analytically a " parcel of energy " of relatively small dimensions, which travels with the speed of light, or when dispersion occurs, with the group velocity. Thereby is given the instantaneous *position* of the parcel of energy—if the detailed structure is not in question—in a very plausible way as that point of space where *all* the superposed plane waves meet in *exactly* agreeing phase.

We will now apply these considerations to the q-space waves. We select, at a definite time t, a definite point P of q-space, through which the parcel of waves passes in a given direction R, at that time. In addition let the mean frequency ν or the mean E-value for the packet be also given. These conditions correspond exactly to postulating that at a given time the mechanical system is starting from a given

[1] P. Debye, *Ann. d. Phys.* 30, p. 755, 1909.

[2] M. v. Laue, *idem* 44, p. 1197 (§ 2), 1914.   [3] *Loc. cit.*

configuration with given velocity components. (Energy *plus* direction is equivalent to velocity components.)

In order to carry over the optical construction, we require firstly *one* set of wave surfaces with the desired frequency, *i.e. one* solution of the Hamilton-Jacobi equation (1′) for the given E-value. This solution, W, say, is to have the following property: the surface of the set which passes through P at time t, which we may denote by

(14) $$W = W_0,$$

must have its normal at P in the prescribed direction R. But this is still not enough. We must be able to vary to an infinitely small extent this set of waves W in an n-fold manner ($n =$ number of degrees of freedom), so that the wave normal will sweep out an infinitely small $(n-1)$ dimensional space angle at the point P, and so that the frequency $\frac{E}{h}$ will vary in an infinitely small *one*-dimensional region, whereby care is taken that all members of the infinitely small n-dimensional continuum of sets of waves meet together at time t in the point P in exactly agreeing phase. Then it is a question of finding at any other time *where* that point lies at which this agreement of phases occurs.

To do this, it will be sufficient if we have at our disposal a solution W of the Hamilton-Jacobi equation, which is dependent not only on the constant E, here denoted by a_1, but also on $(n-1)$ additional constants $a_2, a_3 \ldots a_n$, in such a way that it cannot be written as a function of less than n combinations of these n constants. For then we can, firstly, bestow on a_1 the value prescribed for E, and, secondly, define $a_2, a_3 \ldots a_n$, so that the surface of the set passing through the point P has at P the prescribed normal direction. Henceforth we understand by $a_1, a_2 \ldots a_n$, *these* values, and take (14) as the surface of *this* set, which passes through the point P at time t. Then we consider the *continuum of sets* which belongs to the a_k-values of an adjacent infinitesimal a_k-region. A member of this continuum, *i.e.* therefore *a set*, will be given by

(15) $$W + \frac{\partial W}{\partial a_1} da_1 + \frac{\partial W}{\partial a_2} da_2 + \ldots + \frac{\partial W}{\partial a_n} da_n = \text{const.}$$

for a *fixed* set of values of $da_1, da_2 \ldots da_n$, and varying constant. That member of *this set, i.e.* therefore that single surface, which goes through P at time t will be defined by the following choice of the const.,

(15′) $$W + \frac{\partial W}{\partial a_1} da_1 + \ldots + \frac{\partial W}{\partial a_n} da_n = W_0 + \left(\frac{\partial W}{\partial a_1}\right)_0 da_1 + \ldots + \left(\frac{\partial W}{\partial a_n}\right)_0 da_n,$$

where $\left(\frac{\partial W}{\partial a_1}\right)_0$, etc., are the *constants* obtained by substituting in the differential coefficients the co-ordinates of the point P and the value t of the time $\left(\text{which latter really only occurs in } \frac{\partial W}{\partial a_1}\right)$.

The surfaces (15′) for all possible sets of values of $da_1, da_2 \ldots da_n,$

form on their part *a set*. They all go through the point P at time t, their wave normals continuously sweep out a little $(n-1)$ dimensional solid angle and, moreover, their E-parameter also varies within a small region. The set of surfaces (15′) is so formed that each of the sets (15) supplies *one* representative to (15′), namely, that member which passes through P at time t.

We will now assume that the phase angles of the wave functions which belong to the sets (15) happen to agree precisely for those representatives which enter the set (15′). They agree therefore at time t at the point P.

We now ask: Is there, at *any arbitrary time*, a point where all surfaces of the set (15′) cut one another, *and in which, therefore*, all the wave functions which belong to the sets (15) agree in phase ? The answer is : *There exists* a point of agreeing phase, but it is *not* the common intersection of the surfaces of set (15′), for such does *not* exist at any subsequent arbitrary time. Moreover, the point of phase agreement arises in *such a way* that the sets (15) *continuously exchange* their representatives given to (15′).

That is shown thus. There must hold

$$(16) \qquad W = W_0, \frac{\partial W}{\partial a_1} = \left(\frac{\partial W}{\partial a_1}\right)_0, \frac{\partial W}{\partial a_2} = \left(\frac{\partial W}{\partial a_2}\right)_0 \cdots \frac{\partial W}{\partial a_n} = \left(\frac{\partial W}{\partial a_n}\right)_0,$$

simultaneously for the common meeting point of all members of (15′) at any time, because the da_1's are arbitrary within a small region. In these $n+1$ equations, the right-hand sides are constants, and the left are functions of the $n+1$ quantities $q_1, q_2, \ldots q_n, t$. The equations are satisfied by the initial system of values, *i.e.* by the co-ordinates of P and the initial time t. For another arbitrary value of t, they will have *no* solutions in $q_1 \ldots q_n$, but will *more than define* the system of these n quantities.

We may proceed, however, as follows. Let us leave the first equation, $W = W_0$, aside at first, and define the q_k's as functions of the time and the constants according to the remaining n equations. Let this point be called Q. By it, naturally, the *first* equation will *not* be satisfied, but the left-hand side will differ from the right by a certain value. If we go back to the derivation of system (16) from (15′), what we have just said means that though Q is not a common point for the set of surfaces (15′), it is so, however, for a set which results from (15′), if we alter the right-hand side of equation (15′) by an amount which is constant for all the surfaces. Let this new set be (15″). For it, therefore, Q is a common point. The new set results from (15′), as stated above, by an exchange of the representatives in (15′). This exchange is occasioned by the alteration of the constant in (15), *by the same amount*, for all representatives. Hence the *phase angle* is altered by the same amount for all representatives. The new representatives, *i.e.* the members of the set we have called (15″), which meet in the point Q, agree in phase angle just as the old ones did. This amounts therefore to saying :

The point Q which is defined as a function of the time by the n equations

$$(17) \qquad \frac{\partial W}{\partial a_1} = \left(\frac{\partial W}{\partial a_1}\right)_0, \quad \ldots, \quad \frac{\partial W}{\partial a_n} = \left(\frac{\partial W}{\partial a_n}\right)_0,$$

continues to be a point of agreeing phase for the whole aggregate of wave sets (15).

Of all the n-surfaces, of which Q is shown by (17) to be the common point, only the first is variable; the others remain fixed (only the first of equations (17) contains the time). The $n-1$ fixed surfaces determine the *path* of the point Q as their line of intersection. It is easily shown that this line is the orthogonal trajectory of the set $W = $ const. For, by hypothesis, W satisfies the Hamilton-Jacobi equation (1') identically in $a_1, a_2 \ldots a_n$. If we now differentiate the Hamilton - Jacobi equation with respect to a_k ($k=2, 3, \ldots n$), we get the statement that the normal to a surface, $\frac{\partial W}{\partial a_k} = $ const., is *perpendicular*, at every point on it, to the normal of the surface, $W = $ const., which passes through that point, *i.e.* that each of the two surfaces *contains* the normal to the other. If the line of intersection of the $n-1$ fixed surfaces (17) has no branches, as is generally the case, then must each line element of the intersection, as the *sole common* line element of the $n-1$ surfaces, coincide with the normal of the W-surface, passing through the same point, *i.e.* the line of intersection is the orthogonal trajectory of the W-surfaces. Q.E.D.

We may sum up the somewhat detailed discussion, which has led us to equations (17), in a much shorter or (so to speak) shorthand fashion, as follows: W denotes, apart from a universal constant $\left(\frac{1}{h}\right)$, the phase angle of the wave function. If we now deal not merely with *one*, but with a continuous manifold of wave systems, and if these are continuously arranged by means of any continuous parameters a_i, then the equations $\frac{\partial W}{\partial a_i} = $ const. express the fact that all infinitely adjacent individuals (wave systems) of this manifold agree in phase. These equations therefore define the geometrical locus of the points of agreeing phase. If the equations are sufficient, this locus shrinks to one point; the equations then define *the point* of phase agreement as a function of the time.

Since the system of equations (17) agrees with the known second system of equations of Jacobi, we have thus shown:

The point of phase agreement for certain infinitesimal manifolds of wave systems, containing n *parameters, moves according to the same laws as the image point of the mechanical system.*

I consider it a very difficult task to give an exact proof that the superposition of these wave systems really produces a noticeable disturbance in only a relatively small region surrounding the point of phase agreement, and that everywhere else they practically destroy

one another through interference, or that the above statement turns out to be true at least for a suitable choice of the amplitudes, and possibly for a special choice of the *form* of the wave surfaces. I will advance the physical hypothesis, which I wish to attach to what is to be proved, without attempting the proof. The latter will only be worth while if the hypothesis stands the test of trial *and* if its application should *require* the exact proof.

On the other hand, we may be sure that the region to which the disturbance may be confined still contains in all directions a great number of wave lengths. This is directly evident, firstly, because so long as we are only a *few* wave lengths distant from the point of phase agreement, then the agreement of phase is hardly disturbed, as the interference is still almost as favourable as it is at the point itself. Secondly, a glance at the three-dimensional Euclidean case of ordinary optics is sufficient to assure us of this general behaviour.

What I now categorically conjecture is the following :

The true mechanical process is realised or represented in a fitting way by the *wave processes* in *q*-space, and not by the motion of *image points* in this space. The study of the motion of image points, which is the object of classical mechanics, is only an approximate treatment, and has, as such, just as much justification as geometrical or " ray " optics has, compared with the true optical process. A macroscopic mechanical process will be portrayed as a wave signal of the kind described above, which can approximately enough be regarded as confined to a point compared with the geometrical structure of the path. We have seen that the same laws of motion hold exactly for such a signal or group of waves as are advanced by classical mechanics for the motion of the image point. This manner of treatment, however, loses all meaning where the structure of the path is no longer very large compared with the wave length or indeed is comparable with it. Then we *must* treat the matter strictly on the wave theory, *i.e.* we must proceed from the *wave equation* and not from the fundamental equations of mechanics, in order to form a picture of the manifold of the possible processes. These latter equations are just as useless for the elucidation of the micro-structure of mechanical processes as geometrical optics is for explaining the *phenomena of diffraction*.

Now that a certain interpretation of this micro-structure has been successfully obtained as an addition to classical mechanics, although admittedly under new and very artificial assumptions, an interpretation bringing with it practical successes of the highest importance, it seems to me very significant that these theories—I refer to the forms of quantum theory favoured by Sommerfeld, Schwarzschild, Epstein, and others—bear a very close relation to the Hamilton-Jacobi equation and the theory of its solution, *i.e.* to that form of classical mechanics which already points out most clearly the true undulatory character of mechanical processes. The Hamilton-Jacobi equation corresponds to Huygens' Principle (in its old simple form, not in the form due to Kirchhoff). And just as this, supplemented by

some rules which are not intelligible in geometrical optics (Fresnel's construction of zones), can explain to a great extent the phenomena of diffraction, so light can be thrown on the processes in the atom by the theory of the action-function. But we inevitably became involved in irremovable contradictions if we tried, as was very natural, to maintain also the idea of *paths of systems* in these processes; just as we find the tracing of the course of a *light ray* to be meaningless, in the neighbourhood of a diffraction phenomenon.

We can argue as follows. I will, however, not yet give a conclusive picture of the actual process, which positively cannot be arrived at from this starting-point but only from an investigation of the wave equation; I will merely illustrate the matter qualitatively. Let us think of a wave group of the nature described above, which in some way gets into a small closed " path ", whose dimensions are of the order of the wave length, and therefore *small* compared with the dimensions of the wave group itself. It is clear that then the " system path " in the sense of classical mechanics, *i.e.* the path of the point of exact phase agreement, will completely lose its prerogative, because there exists a whole continuum of points before, behind, and near the particular point, in which there is almost as complete phase agreement, and which describe totally different " paths ". In other words, the wave group not only fills the whole path domain all at once but also stretches far beyond it in all directions.

In *this* sense do I interpret the " phase waves " which, according to de Broglie, accompany the path of the electron; in the sense, therefore, that no special meaning is to be attached to the electronic path itself (at any rate, in the interior of the atom), and still less to the position of the electron on its path. And in this sense I explain the conviction, increasingly evident to-day, *firstly*, that real meaning has to be denied to the *phase* of electronic motions in the atom; *secondly*, that we can never assert that the electron at a definite instant is to be found on *any definite one* of the quantum paths, specialised by the quantum conditions; and *thirdly*, that the true laws of quantum mechanics do not consist of definite rules for the *single path*, but that in these laws the elements of the whole manifold of paths of a system are bound together by equations, so that apparently a certain reciprocal action exists between the different paths.[1]

It is not incomprehensible that a careful analysis of the experimentally known quantities should lead to assertions of this kind, if the experimentally known facts are the outcome of such a structure of the real process as is here represented. All these assertions systematically contribute to the relinquishing of the ideas of " place of the electron " and " path of the electron ". If these are not given up, contradictions remain. This contradiction has been so strongly felt that it has even been. doubted whether what goes on in the atom could ever be described within the scheme of space and time. From the philo-

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[1] Cf. especially the papers of Heisenberg, Born, Jordan, and Dirac quoted later, and further N. Bohr, *Die Naturwissenschaften*, January 1926.

sophical standpoint, I would consider a conclusive decision in this sense as equivalent to a complete surrender. For we cannot really alter our manner of thinking in space and time, and what we cannot comprehend within it we cannot understand at all. There *are* such things—but I do not believe that atomic structure is one of them. From our standpoint, however, there is no reason for such doubt, although or rather *because* its appearance is extraordinarily comprehensible. So might a person versed in geometrical optics, after many attempts to explain diffraction phenomena by means of the idea .of the ray (trustworthy for his macroscopic optics), which always came to nothing, at last think that the *Laws of Geometry* are not applicable to diffraction, since he continually finds that light rays, which he imagines as *rectilinear* and *independent* of each other, now suddenly show, even in homogeneous media, the most remarkable *curvatures*, and obviously *mutually influence* one another. I consider this analogy as *very* strict. Even for the unexplained *curvatures*, the analogy in the atom is not lacking—think of the " non-mechanical force", devised for the explanation of anomalous Zeeman effects.

In what way now shall we have to proceed to the undulatory representation of mechanics for those cases where it is necessary ? We must start, not from the fundamental equations of mechanics, but from a wave equation for *q*-space and consider the manifold of processes possible *according to it*. The wave equation has not been explicitly used or even put forward in this communication. The only datum for its construction is the *wave velocity*, which is given by (6) or (6′) as a function of the mechanical energy parameter or frequency respectively, and by this datum the wave equation is evidently not uniquely defined. It is not even decided that it must be definitely of the second order. Only the striving for simplicity leads us to try this to begin with. We will then say that for the wave function ψ we have

$$(18) \qquad \operatorname{div} \operatorname{grad} \psi - \frac{1}{u^2}\ddot{\psi} = 0,$$

valid for all processes which only depend on the time through a factor $e^{2\pi i\nu t}$. Therefore, considering (6), (6′), and (11), we get, respectively,

$$(18') \qquad \operatorname{div} \operatorname{grad} \psi + \frac{8\pi^2}{h^2}(h\nu - V)\psi = 0,$$

and

$$(18'') \qquad \operatorname{div} \operatorname{grad} \psi + \frac{8\pi^2}{h^2}(E - V)\psi = 0.$$

The differential operations are to be understood with regard to the line element (3). But even under the postulation of second order, the above is not the only equation consistent with (6). For it is possible to generalize by replacing div grad ψ by

$$(19) \qquad f(q_k) \operatorname{div} \left(\frac{1}{f(q_k)} \operatorname{grad} \psi\right),$$

where f may be an arbitrary function of the q's, which must depend in

some plausible way on E, $V(q_k)$, and the coefficients of the line element (3). (Think, *e.g.*, of $f=u$.) Our postulation is again dictated by the striving for simplicity, yet I consider in this case that a wrong deduction is not out of the question.[1]

The substitution of a *partial* differential equation for the equations of dynamics in atomic problems appears at first sight a very doubtful procedure, on account of the multitude of solutions that such an equation possesses. Already classical dynamics had led not just to one solution but to a much too extensive manifold of solutions, viz. to a continuous set, while all experience seems to show that only a discrete number of these solutions is realised. The problem of the quantum theory, according to prevailing conceptions, is to select by means of the "quantum conditions" that discrete set of actual paths out of the continuous set of paths possible according to classical mechanics. It seems to be a bad beginning for a new attempt in this direction if the number of possible solutions has been *increased* rather than diminished.

It is true that the problem of classical dynamics also allows itself to be presented in the form of a *partial* equation, namely, the Hamilton-Jacobi equation. But the manifold of solutions of the problem does not correspond to the manifold of solutions of that equation. An arbitrary "complete" solution of the equation solves the mechanical problem *completely*; any *other* complete solution yields the same paths —they are only contained in another way in the manifold of paths.

Whatever the fear expressed about taking equation (18) as the foundation of atomic dynamics comes to, I will not positively assert that no further additional definitions will be required with it. But these will probably no longer be of such a completely strange and incomprehensible nature as the previous "quantum conditions", but will be of the type that we are accustomed to find in physics with a partial differential equation as initial or boundary conditions. They will be, in no way, *analogous* to the quantum conditions—because in all cases of classical dynamics, which I have investigated up till now, it turns out that equation (18) *carries within itself the quantum conditions.* It distinguishes in certain cases, and indeed in those where experience demands it, *of itself*, certain frequencies or energy levels as those which alone are possible for stationary processes, without any further assumption, other than the almost obvious demand that, as a physical quantity, the function ψ must be single-valued, finite, and continuous throughout configuration space.

Thus the fear expressed is transformed into its contrary, in any case in what concerns the energy levels, or let us say more prudently, the frequencies. (For the question of the "vibrational energy" stands by itself; we must not forget that it is only in the one electron problem that the interpretation as a vibration in real three-dimensional space is immediately suggested.) The definition of the quantum levels *no*

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[1] The introduction of $f(q_k)$ means that not only the "density" but also the "elasticity" varies with the position.

longer takes place in two separated stages : (1) Definition of all paths dynamically possible.   (2) *Discarding* of the greater part of those solutions and the selection of a few by special postulations ; on the contrary, the quantum levels are *at once* defined as the *proper values* of equation (18), which *carries in itself its natural boundary conditions*.

As to how far an analytical simplification will be effected in this way in more complicated cases, I have not yet been able to decide. I should, however, expect so.   Most of the analytical investigators have the feeling that in the two-stage process, described above, there must be yielded in (1) the solution of a more complicated problem than is really necessary for the final result : energy as a (usually) very simple rational function of the quantum numbers.   Already, as is known, the application of the Hamilton-Jacobi method creates a great simplification, as the actual calculation of the mechanical solution is avoided.   It is sufficient to evaluate the integrals, which represent the momenta, merely for a closed complex path of integration instead of for a variable upper limit, and this gives much less trouble.   Still the complete solution of the Hamilton-Jacobi equation must really be known, *i.e.* given by quadratures, so that the integration of the mechanical problem must in principle be effected for arbitrary initial values. In seeking for the proper values of a differential equation, we must usually, in practice, proceed thus.   We seek the solution, firstly, without regard to boundary or continuity conditions, and from the form of the solution then pick out those values of the parameters, for which the solution satisfies the given conditions. Part I. supplies an example of this.   We see by this example also, however—what is typical of proper value problems—that the solution was only given *generally* in an extremely inaccessible analytical form [equation (12) *loc. cit.*], but that it is extraordinarily simplified for those proper values belonging to the " natural boundary condition ".   I am not well enough informed to say whether *direct* methods have now been worked out for the calculation of the proper values. This is known to be so for the distribution of proper values of *high order*. But this limiting case is *not* of interest here ; it corresponds to the classical, macroscopic mechanics.   For spectroscopy and atomic physics, in general just the *first* 5 or 10 proper values will be of interest ; even the *first alone* would be a great result—it defines the *ionisation potential.* From the idea, definitely outlined, that every problem of proper values allows itself to be treated as one of maxima and minima without direct reference to the differential equation, it appears to me very probable that direct methods will be found for the calculation, at least approximately, of the proper values, as soon as *urgent* need arises.   At least it should be possible to test in individual cases whether the proper values, *known* numerically to all desired accuracy through spectroscopy, *satisfy* the problem or not.

I would not like to proceed without mentioning here that at the present time a research is being prosecuted by Heisenberg, Born,

Jordan, and other distinguished workers,[1] to remove the quantum difficulties, which has already yielded such noteworthy success that it cannot be doubted that it contains at least a part of the truth. In its *tendency*, Heisenberg's attempt stands very near the present one, as we have already mentioned. In its method, it is so totally different that I have not yet succeeded in finding the connecting link. I am distinctly hopeful that these two advances will not fight against one another, but on the contrary, just because of the extraordinary difference between the starting-points and between the methods, that they will supplement one another and that the one will make progress where the other fails. The strength of Heisenberg's programme lies in the fact that it promises to give the *line-intensities*, a question that we have not approached as yet. The strength of the present attempt—— —if I may be permitted to pronounce thereon—lies in the guiding, physical point of view, which creates a bridge between the macroscopic and microscopic mechanical processes, and which makes intelligible the outwardly different modes of treatment which they demand. For me, personally, there is a special charm in the conception, mentioned at the end of the previous part, of the emitted frequencies as " beats ", which I believe will lead to an intuitive understanding of the intensity formulae.

§ 3. Application to Examples

We will now add a few more examples to the Kepler problem treated in Part I., but they will only be of the very simplest nature, since we have provisionally confined ourselves to *classical* mechanics, with no magnetic field.[2]

1. *The Planck Oscillator. The Question of Degeneracy*

Firstly we will consider the one-dimensional oscillator. Let the co-ordinate q be the displacement multiplied by the square root of the mass. The two forms of the kinetic energy then are

$$(20) \qquad \bar{T} = \tfrac{1}{2}\dot{q}^2, \quad T = \tfrac{1}{2}p^2.$$

The potential energy will be

$$(21) \qquad V(q) = 2\pi^2 \nu_0^2 q^2,$$

where ν_0 is the proper frequency in the mechanical sense. Then equation (18) reads in this case

$$(22) \qquad \frac{d^2\psi}{dq^2} + \frac{8\pi^2}{h^2}(E - 2\pi^2\nu_0^2 q^2)\psi = 0.$$

[1] W. Heisenberg, *Ztschr. f. Phys.* 33, p. 879, 1925 ; M. Born and P. Jordan, *ibid.* 34, p. 858, 1925 ; M. Born, W. Heisenberg, and P. Jordan, *ibid.* 35, p. 557, 1926 ; P. Dirac, *Proc. Roy. Soc.*, London, 109, p. 642, 1925.

[2] In relativity mechanics and taking a magnetic field into account the statement of the Hamilton-Jacobi equation becomes more complicated. In the case of a single electron, it asserts that the *four-dimensional* gradient of the action function, *diminished* by a given vector (the four-potential), has a constant value. The translation of this statement into the language of the wave theory presents a good many difficulties.

For brevity write

(23)
$$a = \frac{8\pi^2 E}{h^2}, \quad b = \frac{16\pi^4 \nu_0{}^2}{h^2}.$$

Therefore

(22')
$$\frac{d^2\psi}{dq^2} + (a - bq^2)\psi = 0.$$

Introduce as independent variable

(24)
$$x = q\sqrt[4]{b},$$

and obtain

(22")
$$\frac{d^2\psi}{dx^2} + \left(\frac{a}{\sqrt{b}} - x^2\right)\psi = 0.$$

The proper values and functions of this equation are *known*.[1] The proper values are, with the notation used here,

(25)
$$\frac{a}{\sqrt{b}} = 1, 3, 5 \ldots (2n+1) \ldots$$

The functions are the *orthogonal functions of Hermite*,

(26)
$$e^{-\frac{x^2}{2}} H_n(x).$$

$H_n(x)$ means the nth Hermite polynomial, which can be defined as

(27)
$$H_n(x) = (-1)^n e^{x^2} \frac{d^n e^{-x^2}}{dx^n},$$

or explicitly by

(27') $$H_n(x) = (2x)^n - \frac{n(n-1)}{1!}(2x)^{n-2}$$

$$+ \frac{n(n-1)(n-2)(n-3)}{2!}(2x)^{n-4} - + \ldots$$

The first of these polynomials are

(27")
$$H_0(x) = 1 \qquad\qquad H_1(x) = 2x$$
$$H_2(x) = 4x^2 - 2 \qquad\qquad H_3(x) = 8x^3 - 12x$$
$$H_4(x) = 16x^4 - 48x^2 + 12 \ldots$$

Considering next the proper values, we get from (25) and (23)

(25')
$$E_n = \frac{2n+1}{2} h\nu_0 ; \quad n = 0, 1, 2, 3, \ldots$$

Thus as quantum levels appear so-called " half-integral " multiples of the " quantum of energy " peculiar to the oscillator, *i.e.* the *odd* multiples of $\frac{h\nu_0}{2}$. The intervals between the levels, which alone are important for the radiation, are the same as in the former theory. It is remarkable that our quantum levels are *exactly* those of Heisenberg's theory. In the theory of *specific heat* this deviation from the previous

[1] Cf. Courant-Hilbert, *Methods of Mathematical Physics*, i. (Berlin, Springer, 1924), v. § 9, p. 261, eqn. 43, and further ii. § 10, 4, p. 76.

theory is not without significance. It becomes important first when the proper frequency ν_0 *varies* owing to the dissipation of heat. Formally it has to do with the old question of the " zero-point energy ", which was raised in connection with the choice between the first and second forms of Planck's Theory. By the way, the additional term $\frac{h\nu_0}{2}$ also influences the law of the *band-edges*.

The *proper functions* (26) become, if we reintroduce the original q from (24) and (23),

$$(26') \qquad \psi_n(q) = e^{-\frac{2\pi^2\nu_0 q^2}{h}} H_n\left(2\pi q\sqrt{\frac{\nu_0}{h}}\right).$$

Consideration of (27″) shows that the first function is a *Gaussian Error-curve*; the second vanishes at the origin and for x positive corresponds to a " Maxwell distribution of velocities " in two dimensions, and is continued in the manner of an odd function for x negative. The third function is even, is negative at the origin, and has two symmetrical zeros at $\pm\frac{1}{\sqrt{2}}$, etc. The curves can easily be sketched roughly and it is seen that the roots of consecutive polynomials *separate* one another. From (26′) it is also seen that the characteristic points of the proper functions, such as half-breadth (for $n=0$), zeros, and maxima, are, as regards order of magnitude, within the range of the classical vibration of the oscillator. For the classical *amplitude* of the nth vibration is readily found to be given by

$$(28) \qquad q_n = \frac{\sqrt{E_n}}{2\pi\nu_0} = \frac{1}{2\pi}\sqrt{\frac{h}{\nu_0}}\sqrt{\frac{2n+1}{2}}.$$

Yet there is in general, as far as I see, no definite meaning that can be attached to the *exact* abscissa of the classical *turning points* in the graph of the proper function. It may, however, be conjectured, because the turning points have *this* significance for the phase space wave, that, at them, the square of the velocity of propagation becomes *infinite* and at greater distances becomes *negative*. In the differential equation (22), however, this only means the *vanishing* of the coefficient of ψ and gives rise to no singularities.

I would not like to suppress the remark here (and it is valid quite generally, not merely for the oscillator), that nevertheless this vanishing and becoming imaginary of the velocity of propagation is something which is very characteristic. It is the analytical reason for the selection of definite proper values, merely through the condition that the function should remain finite. I would like to illustrate this further. A wave equation with a *real* velocity of propagation means just this : there is an *accelerated* increase in the value of the function at all those points where its value is *lower* than the average of the values at neighbouring points, and vice versa. Such an equation, if not immediately and lastingly as in case of the *equation for the conduction of heat*, yet in the course of time, causes a *levelling*

of extreme values and does not permit at any point an excessive growth of the function. A wave equation with an *imaginary* velocity of propagation means the exact opposite: values of the function above the average of surrounding values experience an *accelerated increase* (or retarded decrease), and vice versa. We see, therefore, that a function represented by such an equation is in the greatest danger of growing beyond all bounds, and we must order matters skilfully to preserve it from this danger. The sharply defined proper values are just what makes this possible. Indeed, we can see in the example treated in Part I. that the demand for sharply defined proper values immediately ceases as soon as we choose the quantity E to be *positive*, as this makes the wave velocity real throughout all space.

After this digression, let us return to the oscillator and ask ourselves if anything is altered when we allow it two or more degrees of freedom (space oscillator, rigid body). If *different* mechanical proper frequencies (ν_0-values) belong to the separate co-ordinates, then nothing is changed. ψ is taken as the *product* of functions, each of a single co-ordinate, and the problem splits up into just as many separate problems of the type treated above as there are co-ordinates present. The proper functions are products of Hermite orthogonal functions, and the proper values of the whole problem appear as sums of those of the separate problems, taken in every possible combination. No proper value (for the whole system) is multiple, if we presume that there is no rational relation between the ν_0-values.

If, however, there is such a relation, then the same manner of treatment is still *possible*, but it is certainly not *unique*. Multiple proper values appear and the "separation" can certainly be effected in other co-ordinates, *e.g.* in the case of the isotropic space oscillator in spherical polars.[1]

The proper values that we get, however, are certainly in each case exactly the same, at least in so far as we are able to prove the "completeness" of a system of proper functions, obtained in *one* way. We recognise here a complete parallel to the well-known relations which the method of the previous quantisation meets with in the case of *degeneracy*. Only in one point there is a not unwelcome formal difference. If we applied the Sommerfeld-Epstein quantum conditions *without* regard to a possible degeneracy then we always got the same energy levels, but reached different conclusions as to the paths permitted, according to the choice of co-ordinates.

Now that is *not* the case here. Indeed we come to a completely different system of proper functions, if we, for example, treat the vibration problem corresponding to unperturbed Kepler motion in

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[1] We are led thus to an equation in r, which may be treated by the method shown in the Kepler problem of Part I. Moreover, the *one*-dimensional oscillator leads to the same equation if q^2 be taken as variable. I originally solved the problem directly in *that* way. For the hint that it was a question of Hermite polynomials, I have to thank Herr E. Fues. The polynomial appearing in the Kepler problem (eqn. 18 of Part I.) is the $(2n+1)$th differential coefficient of the $(n+l)$th polynomial of Laguerre, as I subsequently found.

parabolic co-ordinates instead of the polars used in Part I. However, it is not just the *single proper vibration* that furnishes a *possible state of vibration*, but an arbitrary, finite or infinite, *linear aggregate* of such vibrations. And as such the proper functions found in any second way may always be represented; namely, they may be represented as linear aggregates of the proper functions found in an arbitrary way, provided the latter form a *complete* system.

The question of how the energy is really distributed among the proper vibrations, which has not been taken into account here up till now, will, of course, have to be faced some time. Relying on the former quantum theory, we will be disposed to assume that in the degenerate case only the energy of the set of vibrations belonging to one definite proper value must have a certain prescribed value, which in the non-degenerate case belongs to one single proper vibration. I would like to leave this question still *quite* open—and also the question whether the discovered " energy levels " are really energy steps of the *vibration process* or whether they *merely* have the significance of its frequency. If we accept the beat theory, then the meaning of energy levels is no longer necessary for the explanation of sharp emission frequencies.

2. *Rotator with Fixed Axis*

On account of the lack of potential energy and because of the *Euclidean* line element, this is the simplest conceivable example of vibration theory. Let A be the moment of inertia and ϕ the angle of rotation, then we clearly obtain as the vibration equation

(29)
$$\frac{1}{A}\frac{d^2\psi}{d\phi^2} + \frac{8\pi^2 E}{h^2}\psi = 0,$$

which has the solution

(30)
$$\psi = \frac{\sin}{\cos}\left[\sqrt{\frac{8\pi^2 EA}{h^2}}\cdot\phi\right].$$

Here the argument must be an *integral* multiple of ϕ, simply because otherwise ψ would neither be single-valued nor continuous throughout the range of the co-ordinate ϕ, as we know $\phi + 2\pi$ has the same significance as ϕ. This condition gives the well-known result

(31)
$$E_n = \frac{n^2 h^2}{8\pi^2 A}$$

in *complete* agreement with the former quantisation.

No meaning, however, can be attached to the result of the application to band spectra. For, as we shall learn in a moment, it is a peculiar fact that our theory gives *another* result for the rotator with *free* axis. *And this is true in general.* It is not allowable in the applications of wave mechanics, to think of the freedom of movement of the system as being more strictly limited, in order to simplify calculation, than it *actually is*, even when we know from the integrals of the mechanical

equations that in a single movement certain definite freedoms are not made use of. For micro-mechanics, the fundamental system of mechanical equations is absolutely incompetent; the single paths with which it deals have now no separate existence. A wave process fills the *whole* of the phase space. It is well known that even the *number* of the dimensions in which a wave process takes place is very significant.

3. *Rigid Rotator with Free Axis*

If we introduce as co-ordinates the polar angles θ, ϕ of the radius from the nucleus, then for the kinetic energy as a function of the momenta we get

$$(32) \qquad T = \frac{1}{2A}\left(p_\theta{}^2 + \frac{p_\phi{}^2}{\sin^2\theta}\right).$$

According to its form this is the kinetic energy of a particle constrained to move on a spherical surface. The Laplacian operator is thus simply that part of the spatial Laplacian operator which depends on the polar angles, and the vibration equation (18″) takes the following form,

$$(33) \qquad \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} + \frac{8\pi^2AE}{h^2}\psi = 0.$$

The postulation that ψ should be single-valued and continuous on the spherical surface leads to the proper value condition

$$(34) \qquad \frac{8\pi^2A}{h^2}E = n(n+1); \quad n = 0, 1, 2, 3, \ldots$$

The proper functions are known to be spherical surface harmonics. The energy levels are, therefore,

$$(34') \qquad E_n = \frac{n(n+1)h^2}{8\pi^2A}; \quad n = 0, 1, 2, 3, \ldots$$

This definition is different from all previous statements (except perhaps that of Heisenberg ?). Yet, from various arguments from experiment we were led to put " half-integral " values for n in formula (31). It is easily seen that (34′) gives practically the same as (31) with half-integral values of n. For

$$n(n+1) = (n + \tfrac{1}{2})^2 - \tfrac{1}{4}.$$

The discrepancy consists only of a small additive constant; the level *differences* in (34′) are the same as are got from " half-integral quantisation ". This is true also for the application to short-wave bands, where the moment of inertia is not the same in the initial and final states, on account of the " electronic jump ". For at most a small constant additional part comes in for *all* lines of a band, which is swamped in the large " electronic term " or in the " nuclear vibration term ". Moreover, our previous analysis does not permit us to speak of this small part in any more definite way than as, say,

$$\frac{1}{4}\frac{h^2}{8\pi^2}\left(\frac{1}{A} - \frac{1}{A'}\right).$$

The notion of the moment of inertia being fixed by " quantum conditions " for electronic motions and nuclear vibrations follows naturally from the whole line of thought developed here. We will show in the next section how we can treat, approximately at least, the nuclear vibrations and the rotations of the diatomic molecule simultaneously by a synthesis of the cases [1] considered in 1 and 3.

I should like to mention also that the value $n=0$ corresponds not to the *vanishing* of the wave function ψ but to a *constant* value for it, and accordingly to a vibration with amplitude constant over the whole sphere.

4. *Non-rigid Rotator (Diatomic Molecule)*

According to the observation at the end of section 2, we must state the problem initially with all the six degrees of freedom that the rotator really possesses. Choose Cartesian co-ordinates for the two molecules, viz. x_1, y_1, z_1 ; x_2, y_2, z_2, and let the masses be m_1 and m_2, and r be their distance apart. The potential energy is

$$(35) \qquad V = 2\pi^2 \nu_0^2 \mu (r - r_0)^2,$$

where $\qquad r^2 = (x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2.$

Here

$$(36) \qquad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

may be called the " resultant mass ". Then ν_0 is the mechanical proper frequency of the nuclear vibration, regarding the line joining the nuclei as fixed, and r_0 is the distance apart for which the potential energy is a minimum. These definitions are all in the sense of the usual mechanics.

For the vibration equation (18″) we get the following :

$$(37) \qquad \left\{ \frac{1}{m_1}\left(\frac{\partial^2 \psi}{\partial x_1^2} + \frac{\partial^2 \psi}{\partial y_1^2} + \frac{\partial^2 \psi}{\partial z_1^2}\right) + \frac{1}{m_2}\left(\frac{\partial^2 \psi}{\partial x_2^2} + \frac{\partial^2 \psi}{\partial y_2^2} + \frac{\partial^2 \psi}{\partial z_2^2}\right) \right.$$
$$\left. + \frac{8\pi^2}{h^2}[E - 2\pi^2\nu_0^2\mu(r-r_0)^2]\,\psi = 0. \right.$$

Introduce new independent variables x, y, z, ξ, η, ζ, where

$$(38) \qquad x = x_1 - x_2 ; \quad (m_1 + m_2)\xi = m_1 x_1 + m_2 x_2$$
$$y = y_1 - y_2 ; \quad (m_1 + m_2)\eta = m_1 y_1 + m_2 y_2$$
$$z = z_1 - z_2 ; \quad (m_1 + m_2)\zeta = m_1 z_1 + m_2 z_2.$$

The substitution gives

$$(37') \qquad \left\{ \frac{1}{\mu}\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2}\right) + \frac{1}{m_1 + m_2}\left(\frac{\partial^2 \psi}{\partial \xi^2} + \frac{\partial^2 \psi}{\partial \eta^2} + \frac{\partial^2 \psi}{\partial \zeta^2}\right) \right.$$
$$\left. + [a'' - b'(r-r_0)^2]\,\psi = 0, \right.$$

where for brevity

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[1] Cf. A. Sommerfeld, *Atombau und Spektrallinien*, 4th edit., p. 833. We do not consider here the additional non-harmonic terms in the potential energy.

(39)
$$a'' = \frac{8\pi^2 E}{h^2}, \quad b' = \frac{16\pi^4 \nu_0{}^2 \mu}{h^2}.$$

Now we can put for ψ the product of a function of the relative co-ordinates x, y, z, and a function of the co-ordinates of the centre of mass ξ, η, ζ:

(40)
$$\psi = f(x, y, z)\, g\,(\xi, \eta, \zeta).$$

For g we get the defining equation

(41)
$$\frac{1}{m_1 + m_2}\left(\frac{\partial^2 g}{\partial \xi^2} + \frac{\partial^2 g}{\partial \eta^2} + \frac{\partial^2 g}{\partial \zeta^2}\right) + \text{const. } g = 0.$$

This is of the same form as the equation for the motion, under no forces, of a particle of mass $m_1 + m_2$. The constant would in this case have the meaning

(42)
$$\text{const.} = \frac{8\pi^2 E_t}{h^2},$$

where E_t is the energy of translation of the said particle. Imagine this value inserted in (41). The question as to the values of E_t admissible as proper values depends now on this, whether the whole infinite space is available for the original co-ordinates and hence for those of the centre of gravity without new potential energies coming in, or not. In the first case every non-negative value is permissible and every negative value not permissible. For when E_t is not negative and *only* then, (41) possesses solutions which do not vanish identically and yet remain finite in all space. If, however, the molecule is situated in a " vessel ", then the latter must supply boundary conditions for the function g, or in other words, equation (41), on account of the introduction of further potential energies, will alter its form very abruptly at the walls of the vessel, and thus a discrete set of E_t-values will be selected as proper values. It is a question of the " Quantisation of the motion of translation ", the main points of which I have lately discussed, showing that it leads to Einstein's Gas Theory.[1]

For the factor f of the vibration function ψ, depending on the relative co-ordinates x, y, z, we get the defining equation

(43)
$$\frac{1}{\mu}\left(\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}\right) + [a' - b'(r - r_0)^2]f = 0,$$

where for brevity we put

(39′)
$$a' = \frac{8\pi^2 (E - E_t)}{h^2}.$$

We now introduce instead of x, y, z, the spherical polars r, θ, ϕ (which is in agreement with the previous use of r). After multiplying by μ we get

(43′)
$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 f}{\partial\phi^2}\right\}$$
$$+ [\mu a' - \mu b'(r - r_0)^2]f = 0.$$

[1] *Physik. Ztschr.* 27, p. 95, 1926.

Now break up f. The factor depending on the angles is a surface harmonic. Let the order be n. The curled bracket is $-n(n+1)f$. Imagine this inserted and for simplicity let f now stand for the factor depending on r. Then introduce as new *dependent* variable

(44)
$$\chi = rf,$$

and as new *independent* variable

(45)
$$\rho = r - r_0.$$

The substitution gives

(46)
$$\frac{\partial^2 \chi}{\partial \rho^2} + \left[\mu a' - \mu b' \rho^2 - \frac{n(n+1)}{(r_0 + \rho)^2} \right] \chi = 0.$$

To this point the analysis has been exact. Now we will make an approximation, which I well know requires a stricter justification than I will give here. Compare (46) with equation (22′) treated earlier. They agree in form and only differ in the coefficient of the unknown function by terms of the relative order of magnitude of $\frac{\rho}{r_0}$. This is seen, if we develop thus :

(47)
$$\frac{n(n+1)}{(r_0 + \rho)^2} = \frac{n(n+1)}{r_0^2} \left(1 - \frac{2\rho}{r_0} + \frac{3\rho^2}{r_0^2} - + \ldots \right),$$

substitute in (46), and arrange in powers of ρ/r_0. If we introduce for ρ a new variable differing only by a small constant, viz.

(48)
$$\rho' = \rho - \frac{n(n+1)}{r_0^3 \left(\mu b' + \dfrac{3n(n+1)}{r_0^4} \right)},$$

then equation (46) takes the form

(46′)
$$\frac{\partial^2 \chi}{\partial \rho'^2} + \left(a - b\rho'^2 + \left[\frac{\rho'}{r_0} \right] \right) \chi = 0,$$

where we have put

(49)
$$\begin{cases} a = \mu a' - \dfrac{n(n+1)}{r_0^2} \left(1 - \dfrac{n(n+1)}{r_0^4 \mu b' + 3n(n+1)} \right) \\ b = \mu b' + \dfrac{3n(n+1)}{r_0^4}. \end{cases}$$

The symbol $\left[\dfrac{\rho'}{r_0} \right]$ in (46′) represents terms which are small compared with the retained term of the order of $\dfrac{\rho'}{r_0}$.

Now we know that the *first* proper functions of equation (22′), to which we now compare (46′), only differ markedly from zero in a small range on both sides of the origin. Only those of higher order stretch gradually further out. For moderate orders, the domain for equation (46′), if we *neglect* the term $\left[\dfrac{\rho'}{r_0} \right]$ and bear in mind the

order of magnitude of molecular constants, is indeed small compared with r_0. We thus conclude (without rigorous proof, I repeat), that we can in this way obtain a useful approximation for the first proper functions, within the region where they differ at all markedly from zero, and also for the first *proper values*. From the proper value condition (25) and omitting the abbreviations (49), (39'), and (39), though introducing the small quantity

$$(50) \qquad \epsilon = \frac{n(n+1)h^2}{16\pi^4 \nu_0{}^2 \mu^2 r_0{}^4} = \frac{n(n+1)h^2}{16\pi^4 \nu_0{}^2 A^2}$$

instead, we can easily derive the following *energy steps*,

$$(51) \qquad \begin{cases} E = E_t + \dfrac{n(n+1)h^2}{8\pi^2 A}\left(1 - \dfrac{\epsilon}{1+3\epsilon}\right) + \dfrac{2l+1}{2}h\nu_0\sqrt{1+3\epsilon} \\ (n = 0, 1, 2 \ldots ; \quad l = 0, 1, 2 \ldots), \end{cases}$$

where

$$(52) \qquad\qquad\qquad A = \mu r_0{}^2$$

is still written for the *moment of inertia*.

In the language of classical mechanics, ϵ is the square of the ratio of the frequency of rotation to the vibration frequency ν_0; it is therefore really a small quantity in the application to the molecule, and formula (51) has the usual structure, apart from this small correction and the other differences already mentioned. It is the synthesis of (25') and (34') to which E_t is added as representing the energy of translation. It must be emphasized that the value of the approximation is to be judged not only by the smallness of ϵ but also by l not being too large. *Practically*, however, only small numbers have to be considered for l.

The ϵ-corrections in (51) do *not yet* take account of deviations of the nuclear vibrations from the pure harmonic type. Thus a comparison with Kratzer's formula (*vide* Sommerfeld, *loc. cit.*) and with experience is impossible. I only desired to mention the case provisionally, as an example showing that the intuitive idea of the *equilibrium configuration* of the nuclear system retains its meaning in undulatory mechanics also, and showing the manner in which it does so, provided that the wave amplitude ψ is different from zero practically only in a small neighbourhood of the equilibrium configuration. The direct interpretation of this wave function of *six* variables in *three*-dimensional space meets, at any rate initially, with difficulties of an abstract nature.

The rotation-vibration-problem of the diatomic molecule will have to be re-attacked presently, the non-harmonic terms in the energy of binding *being taken into account*. The method, selected skilfully by Kratzer for the classical mechanical treatment, is also suitable for undulatory mechanics. If, however, we are going to push the calculation as far as is necessary for the fineness of band structure, then we must make use of the theory of the *perturbation of proper values and functions*, that is, of the alteration experienced by a definite proper value and the appertaining proper functions of a

differential equation, when there is added to the coefficient of the unknown function in the equation a small "disturbing term". This "perturbation theory" is the complete counterpart of that of classical mechanics, except that it is simpler because in undulatory mechanics we are always in the domain of *linear* relations. As a first approximation we have the statement that the perturbation of the proper value is equal to the perturbing term averaged "over the undisturbed motion".

The perturbation theory broadens the analytical range of the new theory extraordinarily. As an important practical success, let me say here that the *Stark effect* of the first order will be found to be really completely in accord with Epstein's formula, which has become unimpeachable through the confirmation of experience.