Quantisation as a Problem of Proper Values (Part IV¹)

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ABSTRACT: § 1. Elimination of the energy-parameter from the vibration equation. The real wave equation. Non-conservative systems. § 2. Extension of the perturbation theory to perturbations which explicitly contain the time. Theory of dispersion. § 3. Supplementing § 2. Excited atoms, degenerate systems, continuous spectrum. § 4. Discussion of the resonance case. § 5. Generalisation for an arbitrary perturbation. § 6. Relativistic-magnetic generalisation of the fundamental equations. § 7. On the physical significance of the field scalar.

§ 1. Elimination of the Energy-parameter from the Vibration Equation. The Real Wave Equation. Non-conservative Systems

The wave equation (18) or (18") of Part II., viz.

(1)
$$\nabla^2 \psi - \frac{2(E - V)}{E^2} \frac{\partial^2 \psi}{\partial t^2} = 0$$

or

(1')
$$\nabla^2 \psi + \frac{8\pi^2}{h^2} (E - V) \psi = 0,$$

which forms the basis for the re-establishment of mechanics attempted in this series of papers, suffers from the disadvantage that it expresses the law of variation of the "mechanical field scalar" ψ , neither uniformly nor generally. Equation (1) contains the energy- or frequency-parameter E, and is valid, as is expressly emphasized in Part II., with a definite E-value inserted, for processes which depend on the time exclusively through a definite periodic factor:

(2)
$$\psi \sim \text{real part of } \left(e^{\pm \frac{2\pi i E t}{\hbar}}\right)$$
.

Equation (1) is thus not really any more general than equation (1'),

¹ Cf. Ann. d. Phys. 79, pp. 361, 489; 80, p. 437, 1926 (Parts I., II., III.); further, on the connection with Heisenberg's theory, ibid. 79, p. 734 (p. 45).

which takes account of the circumstance just mentioned and does not contain the time at all.

Thus, when we designated equation (1) or (1'), on various occasions, as "the wave equation", we were really wrong and would have been more correct if we had called it a "vibration-" or an "amplitude-" equation. However, we found it sufficient, because to it is linked the Sturm-Liouville proper value problem—just as in the mathematically strictly analogous problem of the free vibrations of strings

and membranes—and not to the real wave equation.

As to this, we have always postulated up till now that the potential energy V is a pure function of the co-ordinates and does not depend explicitly on the time. There arises, however, an urgent need for the extension of the theory to non-conservative systems, because it is only in that way that we can study the behaviour of a system under the influence of prescribed external forces, e.g. a light wave, or a strange atom flying past. Whenever V contains the time explicitly, it is manifestly impossible that equation (1) or (1') should be satisfied by a function ψ , the method of dependence of which on the time is as given by (2). We then find that the amplitude equation is no longer sufficient and that we must search for the real wave equation.

For conservative systems, the latter is easily obtained. (2) is

equivalent to

(3)
$$\frac{\partial^2 \psi}{\partial t^2} = -\frac{4\pi^2 E^2}{h^2} \psi.$$

We can eliminate E from (1') and (3) by differentiation, and obtain the following equation, which is written in a symbolic manner, easy to understand:

(4)
$$\left(\nabla^2 - \frac{8\pi^2}{h^2}V\right)^2 \psi + \frac{16\pi^2}{h^2} \frac{\partial^2 \psi}{\partial t^2} = 0.$$

This equation must be satisfied by every ψ which depends on the time as in (2), though with E arbitrary, and consequently also by every ψ which can be expanded in a Fourier series with respect to the time (naturally with functions of the co-ordinates as coefficients). Equation (4) is thus evidently the uniform and general wave equation for the field scalar ψ .

It is evidently no longer of the simple type arising for vibrating membranes, but is of the *fourth* order, and of a type similar to that occurring in many problems in the theory of elasticity. However, we need not fear any excessive complication of the theory, or any necessity to revise the previous methods, associated with equation (1'). If V does not contain the time, we can, proceeding from (4), apply (2), and then split up the operator as follows:

(4')
$$\left(\nabla^2 - \frac{8\pi^2}{h^2}V + \frac{8\pi^2}{h^2}E\right)\left(\nabla^2 - \frac{8\pi^2}{h^2}V - \frac{8\pi^2}{h^2}E\right)\psi = 0.$$

¹ E.g., for a vibrating plate, $\nabla^2 \nabla^2 u + \frac{\partial^2 u}{\partial t^2} = 0$. Cf. Courant-Hilbert, chap. v. § 8, p. 256.

By way of trial, we can resolve this equation into two "alternative" equations, namely, into equation (1') and into another, which only differs from (1') in that its proper value parameter will be called minus E, instead of plus E. According to (2) this does not lead to new solutions. The decomposition of (4') is not absolutely cogent, for the theorem that "a product can only vanish when at least one factor vanishes" is not valid for operators. This lack of cogency, however, is a feature common to all the methods of solution of partial differential equations. The procedure finds its subsequent justification in the fact that we can prove the completeness of the discovered proper functions, as functions of the co-ordinates. This completeness, coupled with the fact that the imaginary part as well as the real part of (2) satisfies equation (4), allows arbitrary initial conditions to be fulfilled by ψ and $\partial \psi/\partial t$.

Thus we see that the wave equation (4), which contains in itself the law of dispersion, can really stand as the basis of the theory previously developed for conservative systems. The generalisation for the case of a time-varying potential function nevertheless demands caution, because terms with time derivatives of V may then appear, about which no information can be given to us by equation (4), owing to the way we obtained it. In actual fact, if we attempt to apply equation (4) as it stands to non-conservative systems, we meet with complications, which seem to arise from the term in $\partial V/\partial t$. Therefore, in the following discussions, I have taken a somewhat different route, which is much easier for calculations, and which I consider is justified

in principle.

We need not raise the order of the wave equation to four, in order to get rid of the energy-parameter. The dependence of ψ on the time, which must exist if (1') is to hold, can be expressed by

$$\frac{\partial \psi}{\partial t} = \pm \frac{2\pi i}{\hbar} E \psi$$

as well as by (3). We thus arrive at one of the two equations

(4")
$$\nabla^2 \psi - \frac{8\pi^2}{h^2} V \psi \mp \frac{4\pi i}{h} \frac{\partial \psi}{\partial t} = 0.$$

We will require the complex wave function ψ to satisfy one of these two equations. Since the conjugate complex function $\bar{\psi}$ will then satisfy the other equation, we may take the real part of ψ as the real wave function (if we require it). In the case of a conservative system (4") is essentially equivalent to (4), as the real operator may be split up into the product of the two conjugate complex operators if V does not contain the time.

§ 2. Extension of the Perturbation Theory to Perturbations containing the Time explicitly. Theory of Dispersion

Our main interest is not in systems for which the time and spatial variations of the potential energy V are of the same order of magnitude,

but in systems, conservative in themselves, which are *perturbed* by the addition of small given functions of the time (and of the co-ordinates) to the potential energy. Let us, therefore, write

(5)
$$V = V_0(x) + r(x, t),$$

where, as often before, x represents the whole of the configuration coordinates. We regard the unperturbed proper value problem (r=0) as solved. Then the perturbation problem can be solved by quadratures.

However, we will not treat the general problem immediately, but will select the problem of the dispersion theory out of the vast number of weighty applications which fall under this heading, on account of its striking importance, which really justifies a separate treatment in any case. Here the perturbing forces originate in an alternating electric field, homogeneous and vibrating synchronously in the domain of the atom; and thus, if we have to do with a linearly polarised monochromatic light of frequency ν , we write

(6)
$$r(x,t) = A(x) \cos 2\pi \nu t,$$

and hence

(5')
$$V = V_0(x) + A(x) \cos 2\pi vt.$$

Here A(x) is the negative product of the light-amplitude and the co-ordinate function which, according to ordinary mechanics, signifies the component of the electric moment of the atom in the direction of the electric light-vector (say $-F\Sigma e_i z_i$, if F is the light-amplitude, e_i , z_i the charges and z-co-ordinates of the particles, and the light is polarised in the z-direction). We borrow the time-variable part of the potential function from ordinary mechanics with just as much or as little right as previously, e.g. in the Kepler problem, we borrowed the constant part.

Using (5'), equation (4") becomes

(7)
$$\nabla^2 \psi - \frac{8\pi^2}{h^2} (V_0 + A \cos 2\pi \nu t) \psi \mp \frac{4\pi i}{h} \frac{\partial \psi}{\partial t} = 0.$$

For A = 0, these equations are changed by the substitution

(8)
$$\psi = u(x)e^{\pm \frac{2\pi i E t}{\hbar}}$$

(which is now to be taken in the literal sense, and does not imply pars realis) into the amplitude equation (1') of the unperturbed problem, and we know (cf. § 1) that the totality of the solutions of the unperturbed problem is found in this way. Let

$$E_k \text{ and } u_k(x) ; \quad k=1, 2, 3, \ldots$$

be the proper values and normalised proper functions of the unperturbed problem, which we regard as *known*, and which we will assume to be *discrete* and *different* from one another (non-degenerate system with no continuous spectrum), so that we may not become involved in secondary questions, requiring special consideration.

Just as in the case of a perturbing potential independent of the

time, we will have to seek solutions of the perturbed problem in the neighbourhood of each possible solution of the unperturbed problem, and thus in the neighbourhood of an arbitrary linear combination of the u_k 's, which has constant co-efficients from (8), the u_k 's to be combined with the appropriate time factors $e^{\pm \frac{2\pi i E_k t}{\hbar}}$. The solution of the perturbed problem, lying in the neighbourhood of a definite linear combination, will have the following physical meaning. It will be this solution which first appears, if, when the light wave arrived, precisely that definite linear combination of free proper vibrations was present (perhaps with trifling changes during the "excitation").

Since, however, the equation of the perturbed problem is also homogeneous—let this want of analogy with the "forced vibrations" of acoustics be expressly emphasized—it is evidently sufficient to seek the perturbed solution in the neighbourhood of each separate

$$(9) u_k(x)e^{\pm\frac{2\pi iE_kt}{\hbar}},$$

as we may then linearly combine these ad lib., just as for unperturbed solutions.

To solve the first of equations (7) we therefore now put

(10)
$$\psi = u_k(x)e^{\frac{2\pi i E_k t}{h}} + w(x, t).$$

[The lower symbol, i.e. the second of equations (7), is henceforth left on one side, as it would not yield anything new.] The additional term w(x, t) can be regarded as small, and its product with the perturbing potential neglected. Bearing this in mind while substituting from (10) in (7), and remembering that $u_k(x)$ and E_k are proper functions and values of the unperturbed problem, we get

(11)
$$\begin{cases} \nabla^2 w - \frac{8\pi^2}{h^2} V_0 w - \frac{4\pi i}{h} \frac{\partial w}{\partial t} = \frac{8\pi^2}{h^2} A \cos 2\pi \nu t \cdot u_k e^{\frac{2\pi i E_k t}{h}}, \\ = \frac{4\pi^2}{h^2} A u_k \cdot \left(e^{\frac{2\pi i t}{h} (E_k + h\nu)} + e^{\frac{2\pi i t}{h} (E_k - h\nu)} \right). \end{cases}$$

This equation is readily, and really only, satisfied by the substitution

(12)
$$w = w_{+}(x)e^{\frac{2\pi it}{\hbar}(E_{k}+\hbar\nu)} + w_{-}(x)e^{\frac{2\pi it}{\hbar}(E_{k}-\hbar\nu)},$$

where the two functions w_{\pm} respectively obey the two equations

(13)
$$\nabla^2 w_{\pm} + \frac{8\pi^2}{h^2} (E_k \pm h\nu - V_0) w_{\pm} = \frac{4\pi^2}{h^2} A u_k.$$

This step is essentially unique. At first sight, we apparently can add to (12) an arbitrary aggregate of unperturbed proper vibrations. But this aggregate would necessarily be assumed small, of the first order (since this has been assumed for w), and thus does not interest us at present, as it could only produce perturbations of the second order at most.

In equations (13) we have at last those non-homogeneous equations we might have expected to encounter—in spite of the lack of analogy with real forced vibrations, as emphasized above. This lack of analogy is extraordinarily important and manifests itself in equations (13) in the two following particulars. Firstly, as the "second member" ("exciting force"), the perturbation function A(x) does not appear alone, but multiplied by the amplitude of the free vibration already present. This is indispensable if the physical facts are to be properly taken into account, for the reaction of an atom to an incident light wave depends almost entirely on the state of the atom at that time, whereas the forced vibrations of a membrane, plate, etc., are known to be quite independent of the proper vibrations which may be superimposed on them, and thus would yield an obviously wrong representation of our case. Secondly, in place of the proper value on the left-hand side of (13), i.e. as "exciting frequency", we do not find the frequency v of the perturbing force alone, but rather in one case added to, and in the other subtracted from, that of the free vibration already present. This is equally indispensable. Otherwise the proper frequencies themselves, which correspond to the termfrequencies, would function as resonance-points, and not the differences of the proper frequencies, as is demanded, and is really given by equation (13). Moreover, we see with satisfaction that the latter gives only the differences between a proper frequency which is actually excited and all the others, and not the differences between pairs of proper frequencies, of which no member is excited.

In order to investigate this more closely, let us complete the solution. By well-known methods we find, as simple solutions of

(14)
$$w_{\pm}(x) = \frac{1}{2} \sum_{n=1}^{\infty} \frac{a'_{kn} u_n(x)}{E_k - E_n \pm h^{\nu}},$$

where

(15)
$$a'_{kn} = \int A(x)u_k(x)u_n(x)\rho(x)dx.$$

 $\rho(x)$ is the "density function", i.e. that function of the position-co-ordinates with which equation (1') must be multiplied to make it self-adjoint. The $u_n(x)$'s are assumed to be normalised. It is further postulated that hv does not agree exactly with any of the differences $E_k - E_n$ of the proper values. This "resonance case" will be dealt with later (cf. § 4).

If we now form from (14), using (12) and (10), the entire perturbed vibration, we get

(16)
$$\left\{ \psi = u_k(x)e^{\frac{2\pi iE_k t}{h}} + \frac{1}{2}\sum_{n=1}^{\infty} a'_{kn}u_n(x) \left(\frac{e^{\frac{2\pi it}{h}(E_k + h\nu)}}{E_k - E_n + h\nu} + \frac{e^{\frac{2\pi it}{h}(E_k - h\nu)}}{E_k - E_n - h\nu} \right) \right\}.$$

Thus in the perturbed case, along with each free vibration $u_k(x)$ occur in small amplitude all those vibrations $u_n(x)$, for which $a'_{kn} \neq 0$.

¹ Cf. Part III. §§ 1 and 2, text beside equations (8) and (24).

The latter are exactly those, which, if they exist as free vibrations along with u_k , give rise to a radiation, which is (wholly or partially) polarised in the direction of polarisation of the incident wave. For apart from a factor, a'_{kn} is just the component amplitude, in this direction of polarisation, of the atom's electric moment, which is oscillating with frequency $(E_k - E_n)/h$, according to wave mechanics, and which appears when u_k and u_n exist together. The simultaneous oscillation, however, takes place with neither the proper frequency E_n/h , peculiar to these vibrations, nor the frequency ν of the light wave, but rather with the sum and difference of ν and E_k/h (i.e. the frequency of the one existing free vibration).

The real or the imaginary part of (16) can be considered as the real solution. In the following, however, we will operate with the

complex solution itself.

To see the significance that our result has in the theory of dispersion, we must examine the radiation arising from the simultaneous existence of the excited forced vibrations and the free vibration, already present. For this purpose, we form, following the method we have always adopted above—a criticism follows in § 7—the product of the complex wave function (16) and its conjugate, i.e. the norm of the complex wave function ψ . We notice that the perturbing terms are small, so that squares and products may be neglected. After a simple reduction 3 we obtain

(17)
$$\psi \bar{\psi} = u_k(x)^2 + 2 \cos 2\pi \nu t \sum_{n=1}^{\infty} \frac{(E_k - E_n)a'_{kn}u_k(x)u_n(x)}{(E_k - E_n)^2 - h^2 \nu^2}.$$

According to the heuristic hypothesis on the electrodynamical significance of the field scalar ψ , the present quantity—apart from a multiplicative constant—represents the electrical density as a function of the space co-ordinates and the time, if x stands for only three space co-ordinates, i.e. if we are dealing with the problem of one electron. We remember that the same hypothesis led us to correct selection and polarisation rules and to a very satisfactory representation of intensity relationships in our discussion of the hydrogen Stark effect. By a natural generalisation of this hypothesis—of which more in § 7—we regard the following as representing in the general case the density of the electricity, which is "associated" with one of the particles of classical mechanics, or which "originates in it", or which "corresponds to it in wave mechanics": the integral of $\psi\bar{\psi}$ taken over all those co-ordinates of the system, which in classical mechanics fix the

¹ Cf. what follows, and § 7. ² Cf. end of paper on Quantum Mechanics of Heisenberg, etc., and also the Calculation of Intensities in the Stark Effect in Part III. At the first quoted place, the real part of $\psi\bar{\psi}$ was proposed instead of $\psi\bar{\psi}$. This was a mistake, which was corrected in Part III.

³ We assume as previously, for the sake of simplicity, the proper functions $u_n(x)$ to be *real*, but notice that it may sometimes be much more convenient or even imperative to work with complex aggregates of the real proper functions, e.g. in the proper functions of the Kepler problem to work with $e^{\pm m\phi i}$ instead of $\sin m\phi$.

position of the rest of the particles, multiplied by a certain constant, the classical "charge" of the first particle. The resultant density of charge at any point of space is then represented by the sum of such

integrals taken over all the particles.

Thus in order to find any space component whatever of the total wave-mechanical dipole moment as a function of the time, we must, on this hypothesis, multiply expression (17) by that function of the co-ordinates which gives that particular dipole-component in classical mechanics as a function of the configuration of the point system, e.g. by

$$M_{y} = \sum e_{i}y_{i},$$

if we are dealing with the dipole moment in the y-direction. Then we have to integrate over all the configuration co-ordinates.

Let us work this out, using the abbreviation

(19)
$$b_{kn} = \int M_y(x)u_k(x)u_n(x)\rho(x)dx.$$

Let us elucidate further the definition (15) of the a'_{kn} 's by recalling that if the incident electric light-vector is given by

$$\mathbb{C}_z = F \cos 2\pi \nu t,$$

then

(21)
$$\begin{cases} A(x) = -F \cdot M_z(x), \\ \text{where} \quad M_z(x) = \sum e_i z_i. \end{cases}$$

If we put, in analogy with (19),

(22)
$$a_{kn} = \int M_z(x)u_k(x)u_n(x)\rho(x)dx,$$

then $a'_{kn} = -Fa_{kn}$, and by carrying out the proposed integration we find,

(23)
$$\int M_{\nu} \psi \bar{\psi} \rho dx = a_{kk} + 2F \cos 2\pi \nu t \sum_{n=1}^{\infty} \frac{(E_n - E_k) a_{kn} b_{kn}}{(E_k - E_n)^2 - h^2 \nu^2}$$

for the resulting electric moment, to which the secondary radiation, caused

by the incident wave (20), is to be attributed.

The radiation depends of course only upon the second (time-variable) part, while the first part represents the time-constant dipole moment, which is possibly connected with the originally existing free vibration. This variable part seems fairly promising and may meet all the demands we are accustomed to make on a "dispersion formula". Above all, let us note the appearance of those so-called "negative" terms, which—in the usual phraseology—correspond to the probability of transition to a lower level $(E_n < E_k)$, and to which Kramers 1 was the first to direct attention, from a correspondence

¹ H. A. Kramers, Nature, May 10, 1924; ibid. August 30, 1924; Kramers and W. Heisenberg. Ztschr. f. Phys. 31, p. 681, 1925. The description given in the latter paper of the polarisation of the scattered light (equation 27) from correspondence principles, is almost identical formally with ours.

standpoint. Generally, our formula—despite very different ways of thought and expression—may be characterised as really identical in form with Kramer's formula for secondary radiation. The important connection between a_{kn} , b_{kn} , the coefficients of the secondary and of the spontaneous radiation, is brought out, and indeed the secondary radiation is also described accurately with respect to its condition of polarisation.¹

I would like to believe that the absolute value of the scattered radiation or of the induced dipole moment is also given correctly by formula (23), although it is obviously within the bounds of possibility that an error in the numerical factor may have occurred in applying the heuristic hypothesis introduced above. At any rate the physical dimensions are right, for from (18), (19), (21), and (22) a_{kn} and b_{kn} are electric moments, since the squared integrals of the proper functions were normalised to unity. If ν is far removed from the emission frequency in question, the ratio of the induced to the spontaneous dipole moment is of the same order of magnitude as the ratio of the additional potential energy Fa_{kn} to the "energy step" $E_k - E_n$.

§ 3. Supplements to § 2. Excited Atoms, Degenerate Systems, Continuous Spectrum

For the sake of clearness, we have made some special assumptions, and put many questions aside, in the preceding paragraph. These have

now to be discussed by way of supplement.

First: what happens when the light wave meets the atom, when the latter is in a state in which not merely one free vibration, u_k , is excited as hitherto assumed, but several, say two, u_k and u_l ? As remarked above, we have in the perturbed case simply to combine additively the two perturbed solutions (16) corresponding to the suffix k and the suffix l, after we have provided them with constant (possibly complex) coefficients, which correspond to the strength presumed for the free vibrations, and to the phase relationship of their stimulation. Without actually performing the calculation, we see that in the expression for $\psi\psi$ and also in the expression (23) for the resulting electric moment, there then occurs not merely the corresponding linear aggregate of the terms previously obtained, i.e. of the expressions (17) or (23) written with k, and then with l. We have in addition "combination terms", namely, considering first the greatest order of magnitude, a term in

(24)
$$u_k(x)u_l(x)e^{\frac{2\pi i}{\hbar}(E_k-E_l)t},$$

which gives again the spontaneous radiation, bound up with the co-

¹ It is hardly necessary to say that the two directions which, for simplicity, we have designated as "z-direction" and "y-direction" do not require to be exactly perpendicular to one another. The one is the direction of polarisation of the incident wave; the other is that polarisation component of the secondary wave, in which we are specially interested.

existence of the two free vibrations; and secondly perturbing terms of the first order, which are proportional to the perturbing field amplitude, and which correspond to the interaction of the forced vibrations belonging to u_k with the free vibration u_l —and of the forced vibrations belonging to u_l with u_k . The frequency of these new terms appearing in (17) or (23) is not ν but

$$(25) | \nu \pm (E_k - E_l)/h |,$$

as can easily be seen, still without carrying out the calculation. (New "resonance denominators", however, do not occur in these terms.) Thus we have to do here with a secondary radiation, whose frequency neither coincides with the exciting light-frequency nor with a spontaneous frequency of the system, but is a combination frequency of both.

The existence of this remarkable kind of secondary radiation was first postulated by Kramers and Heisenberg (loc. cit.), from correspondence considerations, and then by Born, Heisenberg, and Jordan from consideration of Heisenberg's quantum mechanics. As far as I know, it has not yet been demonstrated experimentally. The present theory also shows distinctly that the occurrence of this scattered radiation is dependent on special conditions, which demand researches expressly arranged for the purpose. Firstly, two proper vibrations u_k and u_l must be strongly excited, so that all experiments made on atoms in their normal state—as happens in the vast majority of cases—are to be rejected. Secondly, at least one third state of proper vibration must exist (i.e. must be possible—it need not be excited), which leads to powerful spontaneous emission, when combined with u_k as well as with u_k . For the extraordinary scattered radiation, which is to be discovered, is proportional to the product of the spontaneous emission coefficients in question $(a_{kn}b_{ln} \text{ and } a_{ln}b_{kn})$. The combination (u_k, u_l) need not, in itself, cause a strong emission. It would not matter if—to use the language of the older theory—this was a "forbidden transition". Yet in practice we must also demand that the line (u_k, u_l) should actually be emitted strongly during the experiment, for this is the only means of assuring ourselves that both proper vibrations are strongly excited in the same individual atoms and in a sufficiently great number of them. If we reflect now that in the powerful term-series mostly examined, i.e. in the ordinary s-, p-, d-, f-series, the relations are generally such that two terms, which combine strongly with a third, do not do so with one another, then a special choice of the object and conditions of the research seems really necessary, if we are to expect the desired scattered radiation with any certainty, especially as its frequency is not that of the exciting light and thus it does not produce dispersion or rotation of the plane of polarisation, but can only be observed as light scattered on all sides.

As far as I see, the above-mentioned dispersion theory of Heisenberg, Born, and Jordan does not allow of such reflections as we

¹ Born, Heisenberg, and Jordan, Zischr. f. Phys. 35, p. 572, 1926.

have just made, in spite of its great formal similarity to the present one. For it only considers one way in which the atom reacts to incident radiation. It conceives the atom as a timeless entity, and up till now is not able to express in its language the undoubted fact that the atom can be in different states at different times, and thus, as has been proved, reacts in different ways to incident radiation.¹

Let us turn now to another question. In § 2 the collective proper values were postulated to be discrete and different from one another. We now drop the second hypothesis and ask: what is altered when multiple proper values occur, i.e. when degeneracy is present? Perhaps we expect that complications then arise, similar to those we met in the case of a time-constant perturbation (Part III. § 2), i.e. that a system of proper functions of the unperturbed atom, suited to the particular perturbation, must be defined by the solution of a "secular equation", and applied to carry out the perturbation calculation. This is indeed so in the case of an arbitrary perturbation, represented by r(x, t) as in equation (5), but not so in the case of a perturbation by a light wave (equation (6))—at any rate, for our usual first approximation, and as long as we suppose that the light frequency ν does not coincide with any of the spontaneous emission frequencies considered. Then the parameter value in the double equation (13), for the amplitudes of the perturbed vibrations, is not a proper value, and the pair of equations has always the unambiguous pair of solutions (14), in which no vanishing denominators occur even when E_k is a multiple value. Thus the terms in the sum for which $E_n = E_k$ are not, as might be thought, to be omitted, any more than the term for n=k itself. It is worth noticing that through these terms-if one of them occurs really, i.e. with nonvanishing a_{kn} —the frequency $\nu=0$ also appears among the resonance frequencies. These terms do not, of course, contribute to the "ordinary" scattered radiation, as we see from (23), since $E_k - E_n = 0$.

The simplification, that we do not require to consider specially any possible degeneracy present, at least in a first approximation, is always available 2 when the time-averaged value of the perturbation function vanishes, or what is the same thing, when the latter's Fourier expansion in terms of the time contains no constant, i.e. time-

independent, term. This is the case for a light wave.

While our first postulation about the proper values—that they should be simple—has thus shown itself to be really a superfluous precaution, a dropping of the second—that they should be absolutely discrete—while leading to no alterations in principle, brings about, however, very considerable alterations in the external appearance of the calculation, inasmuch as integrals taken over the continuous spectrum of equation (1') are to be added to the discrete sums in (14), (16), (17), and (23). The theory of such representations by integrals has been

¹ Cf. especially the concluding words of Heisenberg's latest exposition of his theory, Math. Ann. 95, p. 683, 1926, in connection with this difficulty of comprehending the course of an event in time.

² Further discussed in § 5.

developed by H. Weyl, and though only for ordinary differential equations, the extension to partials is permissible. In all brevity, the state of the case is this. If the homogeneous equation belonging to the non-homogeneous equations (13), i.e. the vibration equation (1') of the unperturbed system, possesses in addition to a point-spectrum a continuous one, which stretches, say, from E=a to E=b, then an arbitrary function f(x) naturally cannot be developed thus,

(26)
$$f(x) = \sum_{n=1}^{\infty} \phi_n \cdot u_n(x), \quad \text{where } \phi_n = \int f(x) u_n(x) \rho(x) dx$$

in terms of the normalised discrete proper functions $u_n(x)$ alone, but there must be added an integral expansion in terms of the proper solutions u(x, E), which belong to the proper values $a \le E \le b$, and so we have

(27)
$$f(x) = \sum_{n=1}^{\infty} \phi_n \cdot u_n(x) + \int_a^b u(x, E) \phi(E) dE,$$

where to emphasize the analogy we have intentionally chosen the same letter for the "coefficient function" $\phi(E)$ as for the discrete coefficients ϕ_n . If now we have normalised, once for all, the proper solution u(x, E) by associating with it a suitable function of E, in such a way that

(28)
$$\int dx \rho(x) \int_{E'}^{E' + \Delta} u(x, E) u(x, E') dE' = 1 \text{ or } = 0$$

according to whether E belongs to the interval E', $E' + \Delta$ or not, then in (27) under the integral sign we substitute from

(29)
$$\phi(E) = \lim_{\Delta \to 0} \frac{1}{\Delta} \int \rho(\xi) f(\xi) \cdot \int_{E}^{E+\Delta} u(\xi, E') dE' \cdot d\xi,$$

wherein the first integral sign refers as always to the domain of the group of variables x. Assuming (28) to be fulfilled and expansion (27) to exist—which statements are proved by Weyl for ordinary differential equations—the definition of the "coefficient functions" from (29) is almost as obvious as the well-known definition of the Fourier coefficients.

The most important and difficult task in any concrete case is the carrying out of the normalisation of u(x, E), i.e. the finding of that function of E by which we have to multiply the (as yet not normalised) proper solution of the continuous spectrum, in order that condition (28) may be satisfied. The above-quoted works of Herr Weyl contain very valuable guidance for this practical task, and also

¹ H. Weyl, Math. Ann. 68, p. 220, 1910; Gött. Nachr. 1910. Cf. also E. Hilb, Sitz.-Ber. d. Physik. Mediz. Soc. Erlangen, 43, p. 68, 1911; Math. Ann. 71, p. 76, 1911. I have to thank Herr Weyl not only for these references but also for very valuable oral instruction in these not very simple matters.

² I have to thank Herr Fues for this exposition. ³ As Herr E. Fues informs me, we can very often omit the limiting process in practice and write $u(\xi, E)$ for the inner integral, viz. always, when $\int \rho(\xi) f(\xi)u(\xi, E)d\xi$ exists.

some worked-out examples. An example from atomic dynamics on the intensities of band spectra is worked out by Herr Fues in a paper

appearing in the present issue of Annalen der Physik.

Let us apply this to our problem, i.e. to the solution of the pair of equations (13) for the amplitudes w_{\pm} of the perturbed vibrations, where we postulate as usual that the one excited free vibration, u_k , belongs to the discrete point-spectrum. We develop the right-hand side of (13) according to the scheme (27) thus,

(30)
$$\frac{4\pi^2}{h^2}A(x)u_k(x) = \frac{4\pi^2}{h^2}\sum_{n=1}^{\infty} a'_{kn}u_n(x) + \frac{4\pi^2}{h^2}\int_a^b u(x, E)a'_k(E)dE,$$

in which a'_{kn} is given by (15), and $a'_{k}(E)$ from (29) by

(15')
$$a'_k(E) = \lim_{\Delta \to 0} \frac{1}{\Delta} \int \rho(\xi) A(\xi) u_k(\xi) \cdot \int_E^{E+\Delta} u(\xi, E') dE' \cdot d\xi.$$

If we imagine expansion (30) put into (13), and then expand also the desired solution $w_{\pm}(x)$ similarly in terms of the proper solutions $u_n(x)$ and u(x, E), and notice that for the last-named functions the left side of (13) takes the value

$$\frac{8\pi^2}{h^2}(E_k \pm h\nu - E_n)u_n(x)$$

or

$$\frac{8\pi^2}{h^2}(E_k \pm h\nu - E)u(x, E),$$

then by "comparison of coefficients" we obtain as the generalisation of (14)

(14')
$$w_{\pm}(x) = \frac{1}{2} \sum_{n=1}^{\infty} \frac{a'_{kn}u_n(x)}{E_k - E_n \pm h\nu} + \frac{1}{2} \int_a^b \frac{a'_k(E)u(x, E)}{E_k - E \pm h\nu} dE.$$

The further procedure is completely analogous to that of § 2. Finally, we get as additional term for (23)

(23') +2 cos
$$2\pi\nu t \int d\xi \rho(\xi) M_{\nu}(\xi) u_{k}(\xi) \int_{a}^{b} \frac{(E_{k}-E)\alpha'_{k}(E)u(\xi,E)}{(E_{k}-E)^{2}-h^{2}\nu^{2}} dE$$
.

Here, perhaps, we may not always change the order of integration without further examination, because the integral with respect to ξ may possibly not converge. However, we can—as an intuitive makeshift for a strict passage to the limit, which may be dispensed with here—decompose

the integral \int_a^b into many small parts, each having a range Δ , which is

sufficiently small to allow us to regard all the functions of E in question as constant in each part, with the exception of u(x, E), for we know from the general theory that its integral cannot be obtained through such a fixed partition, which is independent of ξ . We can then take the remaining functions out of the partial integrals, and as additional term for the dipole moment (23) of the secondary radiation, obtain finally exactly the following,

(23")
$$2F\cos 2\pi\nu t \int_{a}^{b} \frac{(E-E_{k})a_{k}(E)\beta_{k}(E)}{(E_{k}-E)^{2}-h^{2}\nu^{2}} dE,$$

where

(22')
$$\alpha_k(E) = \lim_{\Delta \to 0} \frac{1}{\Delta} \int \rho(\xi) M_z(\xi) u_k(\xi) \cdot \int_E^{E+\Delta} u(\xi, E') dE' \cdot d\xi,$$

(19')
$$\beta_k(E) = \lim_{\Delta \to 0} \frac{1}{\Delta} \int \rho(\xi) M_{\nu}(\xi) u_k(\xi) \cdot \int_E^{E+\Delta} u(\xi, E') dE' \cdot d\xi$$

(please note the complete analogy with the formulae with the same numbers but without the dashes in § 2).

The preceding sketch of the calculation is of course only a general outline, given merely to show that the much-discussed influence of the continuous spectrum on dispersion, which experiment appears to indicate as existing, is required by the present theory exactly in the form expected, and to outline the way in which the calculation of the problem is to be tackled.

§ 4. Discussion of the Resonance Case

Up till now we have always assumed that the frequency ν of the light wave does not agree with any of the emission frequencies that have to be considered. We now assume that, say,

$$(31) h\nu = E_n - E_k > 0,$$

and we revert, moreover, to the limiting conditions of § 2 for the sake of simplicity (simple, discrete proper values, one single free vibration u_k excited). In the pair of equations (13), the proper value parameter then takes the values

$$(32) E_k \pm E_n \mp E_k = \begin{cases} E_n \\ 2E_k - E_n, \end{cases}$$

i.e. for the upper sign there appears a proper value, namely, E_n . The two cases are possible. Firstly, the right side of equation (13) multiplied by $\rho(x)$, may be orthogonal to the proper function $u_n(x)$ corresponding to E_n , i.e. we have

(33)
$$\int A(x)u_k(x)u_n(x)\rho(x)dx = a'_{kn} = 0,$$

which means, physically, that if u_k and u_n exist together as free vibrations they will give rise to no spontaneous emission or to one which is polarised perpendicularly to the direction of polarisation of the incident light. In this case the critical equation (13) also again possesses a solution, which now, as before, is given by (14), in which the catastrophic term vanishes. This means physically—in the old phraseology—that a "forbidden transition" cannot be stimulated through resonance, or that a "transition", even if not forbidden,

¹ K. F. Herzfeld and K. L. Wolf, Ann. d. Phys. 76, p. 71, 567, 1925; H. Kollmann and H. Mark, Die Nw. 14, p. 648, 1926.

cannot be caused by light which is vibrating perpendicularly to the direction of polarisation of that light which would be emitted

by the "spontaneous transition".

Otherwise, secondly, (33) is not fulfilled. Then the critical equation possesses no solution. Statement (10), which assumes a vibration which differs very little-by quantities of the order of the light amplitude F-from the originally existing free vibration, and is the most general possible under this assumption, thus does not then lead to the goal. No solution, therefore, exists which only differs by quantities of the order of F from the original free vibration. The incident light has thus a varying influence on the state of the system, which bears no relation to the magnitude of the light amplitude. What influence? We can judge this, still without further calculation, if we start out from the case where the resonance condition (31) is not exactly but only approximately fulfilled. Then we see from (16) that $u_n(x)$ is excited in unusually strong forced vibrations, on account of the small denominator, and that—not less important the frequency of these forced vibrations approaches the natural proper frequency E_n/h of the proper vibration u_n . (All this is, indeed, very similar to, yet in a way of its own different from, the resonance phenomena encountered elsewhere; otherwise I would not discuss it so minutely.)

In a gradual approach to the critical frequency, the proper vibration u_n , formerly not excited, whose possible existence is responsible for the crisis, is stimulated to a stronger and stronger degree, and with a frequency more and more closely approaching its own proper frequency. In contradistinction to ordinary resonance phenomena there comes a point, and that even before the critical frequency is reached, where our solution does not represent the circumstances correctly any longer, even under the assumption that our obviously "undamped" wave postulation is strictly correct. For we have in fact regarded the forced vibration w as small compared with the existing free vibration and neglected a squared term

(in equation (11)).

I believe that the present discussion has already shown, with sufficient clearness, that in the resonance case the theory will actually give the result it ought to give, in order to agree with Wood's resonance phenomenon: an increase of the proper vibration u_n , which causes the crisis, to a finite magnitude comparable with that of the originally existing u_k , from which, of course, "spontaneous emission" of the spectral line (u_k, u_n) results. I do not wish, however, to attempt to work out the calculation of the resonance case fully here, because the result would be of little value, so long as the reaction of the emitted radiation on the emitting system is not taken into account. Such a reaction must exist, not only because there is no ground at all for differentiating on principle between the light wave which is incident from outside, and that which is emitted by the system itself, but also because otherwise, if several proper

vibrations were simultaneously excited in a system left to itself, the spontaneous emission would continue indefinitely. This required back-coupling must act so that in this case, along with the light emission, the higher proper vibrations gradually die down, and, finally, the fundamental vibration, corresponding to the normal state of the system, alone remains. The back-coupling is evidently exactly analogous to the reaction of radiation $\left(\frac{2e^2}{3mc^3}\ddot{v}\right)$ in the classical electron theory.

This analogy also allays the increasing apprehension caused by the previous neglect of this back-coupling. The influence of the relevant term (probably no longer linear) in the wave equation will generally be small, just as in the electron the back pressure of radiation is generally very small compared with the force of inertia and the external field strength. In the resonance case, however—just as in the electron theory—the coupling with the proper light wave will be of the same order as that with the incident wave, and must be taken into account, if the "equilibrium" between the different proper vibrations, which

Let it be expressly remarked, however, that the back-coupling term is not necessary for averting a resonance catastrophe! Such can never occur in any circumstances, because according to the theorem of the persistence of normalisation, proved below in § 7, the configuration space integral of $\psi\bar{\psi}$ always remains normalised to the same value, even under the influence of arbitrary external forces—and indeed quite automatically, as a consequence of the wave equation (4"). The amplitudes of the ψ -vibrations, therefore, cannot grow indefinitely; they have, "on the average", always the same value. If one proper vibration waxes, then another must, therefore, wane.

§ 5. Generalisation for an Arbitrary Perturbation

If an arbitrary perturbation is in question as was assumed in equation (5) at the beginning of § 2, then we shall expand the perturbation energy r(x,t) as a Fourier series or Fourier integral in terms of the time. The terms of this expansion have, then, the form (6) of the perturbation potential of a light wave. We see immediately that on the right-hand side of equation (11) we then simply get two series (or, possibly, integrals) of imaginary powers of e, instead of merely two terms. If none of the exciting frequencies coincide with a critical frequency, we get the solution in exactly the same way as described in § 2, but, naturally, as Fourier series (or possibly Fourier integrals) of the time. It serves no purpose to write down the formal expansions here, and a more exact working out of separate problems lies outside the scope of the present paper. Yet an important point, already touched upon in § 3, must be mentioned.

Among the critical frequencies of equation (13), the frequency $\nu = 0$, from $E_k - E_k = 0$, also generally figures. For in this case also one proper value, namely, E_k , appears on the left side as proper value

parameter. Thus, if the frequency 0, i.e. a term independent of the time, occurs in the Fourier expansion of the perturbation function r(x, t), we cannot reach our goal by exactly the earlier method. We easily see, however, how it must be modified, for the case of a time-constant perturbation is known from previous work (cf. Part III.). We have then to consider, at the same time, a small alteration and possibly a splitting up of the proper value or values of the excited free vibrations, i.e. in the indices of the powers of e in the first term on the right hand of equation (10) we have to replace E_k by E_k plus a small constant, the perturbation of the proper value. described in Part III., § 1 and § 2, this perturbation is defined by the postulation that the right side of the critical Fourier component of our equation (13) is to be orthogonal to u_k (or possibly to all the

proper functions belonging to E_k).

The number of special problems, which fall under the question formulated in the present paragraph, is extraordinarily great. By superposing the perturbations due to a constant electric or magnetic field and a light wave, we obtain magnetic and electric double refraction, and magnetic rotation of the plane of polarisation. radiation in a magnetic field also comes under this heading, but for this purpose we must first obtain an exact solution for the resonance case discussed in § 4. Further, we can treat the action of an a-particle or electron flying past the atom 1 in this way, if the encounter is not too close for the perturbation of each of the two systems to be calculable from the undisturbed motion of the other. All these questions are mere matters of calculation as soon as the proper values and functions of the unperturbed systems are known. It is, therefore, to be hoped that we will succeed in defining these functions, at least approximately, for heavier atoms also, in analogy with the approximate definition of the Bohr electronic orbits which belong to different types of terms.

\S 6. Relativistic-magnetic Generalisation of the Fundamental Equations

As an appendix to the physical problems just mentioned, in which the magnetic field, which has hitherto been completely ignored in this series of papers, plays an important part, I would like to give, briefly, the probable relativistic-magnetic generalisation of the basic equations (4"), although I can only do this meantime for the one electron problem, and only with the greatest possible reserve—the latter for two reasons. Firstly, the generalisation is provisionally based on a purely formal analogy. Secondly, as was mentioned in Part I., though it does formally lead in the Kepler problem to Sommerfeld's fine-structure formula with, in fact, the "half-integral" azimuthal and radial quantum, which is generally regarded as correct to-day,

¹ A very interesting and successful attempt to compare the action of flying charged particles with the action of light waves, through a Fourier decomposition of their field, is to be found in a paper by E. Fermi, Zischr. f. Phys. 29, p. 315, 1924.

nevertheless there is still lacking the supplement, which is necessary to secure numerically correct diagrams of the splitting up of the hydrogen lines, and which is given in Bohr's theory by Goudsmit and Uhlenbeck's electronic spin.

The Hamilton-Jacobi partial differential equation for the

Lorentzian electron can readily be written:

$$(34) \begin{cases} \left(\frac{1}{c}\frac{\partial W}{\partial t} + \frac{e}{c}V\right)^{2} - \left(\frac{\partial W}{\partial x} - \frac{e}{c}\mathfrak{A}_{x}\right)^{2} - \left(\frac{\partial W}{\partial y} - \frac{e}{c}\mathfrak{A}_{y}\right)^{2} \\ - \left(\frac{\partial W}{\partial z} - \frac{e}{c}\mathfrak{A}_{z}\right)^{2} - m^{2}c^{2} = 0. \end{cases}$$

Here e, m, c are the charge and mass of the electron, and the velocity of light; V, $\mathfrak A$ are the electro-magnetic potentials of the external electro-magnetic field at the position of the electron, and W is the action function.

From the classical (relativistic) equation (34) I am now attempting to derive the wave equation for the electron, by the following purely formal procedure, which, we can verify easily, will lead to equations (4"), if it is applied to the Hamiltonian equation of a particle moving in an arbitrary field of force in ordinary (non-relativistic) mechanics. After the squaring, in equation (34), I replace the quantities

(35)
$$\begin{cases} \frac{\partial W}{\partial t}, & \frac{\partial W}{\partial x}, & \frac{\partial W}{\partial y}, & \frac{\partial W}{\partial z}, \\ \text{by the respective operators} \\ \pm \frac{h}{2\pi i} \frac{\partial}{\partial t}, & \pm \frac{h}{2\pi i} \frac{\partial}{\partial x}, & \pm \frac{h}{2\pi i} \frac{\partial}{\partial y}, & \pm \frac{h}{2\pi i} \frac{\partial}{\partial z}. \end{cases}$$

The double linear operator, so obtained, is applied to a wave function ψ and the result put equal to zero, thus:

(36)
$$\nabla^{2}\psi - \frac{1}{c^{2}} \frac{\partial^{2}\psi}{\partial t^{2}} \mp \frac{4\pi i e}{hc} \left(\frac{V}{c} \frac{\partial \psi}{\partial t} + \mathfrak{A} \operatorname{grad} \psi \right) + \frac{4\pi^{2}e^{2}}{h^{2}c^{2}} \left(V^{2} - \mathfrak{A}^{2} \frac{m^{2}c^{4}}{e^{2}} \right) \psi = 0.$$

(The symbols ∇^2 and grad have here their elementary three-dimensional Euclidean meaning.) The pair of equations (36) would be the possible relativistic-magnetic generalisation of (4") for the case of a single electron, and should likewise be understood to mean that the complex wave function has to satisfy either the one or the other equation.

From (36) the fine structure formula of Sommerfeld for the hydrogen atom may be obtained by exactly the same method as is described in Part I., and also we may derive (neglecting the term in \mathfrak{A}^2) the normal Zeeman effect as well as the well-known selection and polarisation rules and intensity formulae. They follow from the integral relations between Legendre functions introduced at the end of Part III.

For the reasons given in the first section of this paragraph, I

withhold the detailed reproduction of these calculations meantime, and also in the following final paragraph refer to the "classical", and not to the still incomplete relativistic-magnetic version of the theory.

§ 7. On the Physical Significance of the Field Scalar

The heuristic hypothesis of the electro-dynamical meaning of the field scalar ψ , previously employed in the one-electron problem, was extended off-hand to an arbitrary system of charged particles in § 2, and there a more exhaustive description of the procedure was promised. We had calculated the density of electricity at an arbitrary point in space as follows. We selected one particle, kept the trio of co-ordinates that describes its position in ordinary mechanics fixed; integrated $\psi\bar{\psi}$ over all the rest of the co-ordinates of the system and multiplied the result by a certain constant, the "charge" of the selected particle; we did a similar thing for each particle (trio of co-ordinates), in each case giving the selected particle the same position, namely, the position of that point of space at which we desired to know the electric density. The latter is equal to the algebraic sum of the partial results.

This rule is now equivalent to the following conception, which allows the true meaning of ψ to stand out more clearly. $\psi\bar{\psi}$ is a kind of weight-function in the system's configuration space. wave-mechanical configuration of the system is a superposition of many, strictly speaking of all, point-mechanical configurations kinematically possible. Thus, each point-mechanical configuration contributes to the true wave-mechanical configuration with a certain weight, which is given precisely by $\psi \bar{\psi}$. If we like paradoxes, we may say that the system exists, as it were, simultaneously in all the positions kinematically imaginable, but not "equally strongly" in all. In macroscopic motions, the weight-function is practically concentrated in a small region of positions, which are practically indistinguishable. The centre of gravity of this region in configuration space travels over distances which are macroscopically perceptible. In problems of microscopic motions, we are in any case interested also, and in certain cases even mainly, in the varying distribution over the region.

This new interpretation may shock us at first glance, since we have often previously spoken in such an intuitive concrete way of the " ψ -vibrations" as though of something quite real. But there is something tangibly real behind the present conception also, namely, the very real electrodynamically effective fluctuations of the electric space-density. The ψ -function is to do no more and no less than permit of the totality of these fluctuations being mastered and surveyed mathematically by a single partial differential equation. We have repeatedly called attention 1 to the fact that the ψ -function itself cannot and may not be interpreted directly in terms of three-dimensional space—however much the one-electron problem tends to mislead us on this point—

¹ End of Part II. (p. 39); paper on Heisenberg's quantum mechanics (p. 60).

because it is in general a function in configuration space, not real

space.

Concerning such a weight-function in the above sense, we would wish its integral over the whole configuration space to remain constantly normalised to the same unchanging value, preferably to unity. We can easily verify that this is necessary if the total charge of the system is to remain constant on the above definitions. Even for non-conservative systems, this condition must obviously be postulated. For, naturally, the charge of a system is not to be altered when, e.g., a light wave falls on it, continues for a certain length of time, and then ceases. (N.B.—This is also valid for ionisation processes. A disrupted particle is still to be included in the system, until the separation is also logically—by decomposition of configuration space—completed.)

The question now arises as to whether the postulated persistence of normalisation is actually guaranteed by equations (4''), to which ψ is subject. If this were not the case, our whole conception would practically break down. Fortunately, it is the case. Let us form

(37)
$$\frac{d}{dt} \int \psi \bar{\psi} \rho dx = \int \left(\psi \frac{\partial \bar{\psi}}{\partial t} + \bar{\psi} \frac{\partial \psi}{\partial t} \right) \rho dx.$$

Now, ψ satisfies one of the two equations (4"), and $\bar{\psi}$ the other. Therefore, apart from a multiplicative constant, this integral becomes

(38)
$$\int (\psi \nabla^2 \bar{\psi} - \bar{\psi} \nabla^2 \psi) \rho dx = 2i \int (J \nabla^2 R - R \nabla^2 J) \rho dx,$$

where for the moment we put

$$\psi = R + iJ$$
.

According to Green's theorem, integral (38) vanishes identically; the sole necessary condition that functions R and J must satisfy for this—vanishing in sufficient degree at infinity—means physically nothing more than that the system under consideration should practically be confined to a *finite* region.

We can put this in a somewhat different way, by not immediately integrating over the whole configuration space, but by merely changing the time-derivative of the weight-function into a divergence by Green's transformation. Through this we get an insight into the question of the flow of the weight-function, and thus of electricity. The two equations

$$\frac{\partial \psi}{\partial t} = \frac{h}{4\pi i} \left(\nabla^2 - \frac{8\pi^2}{h^2} V \right) \psi$$

$$\frac{\partial \bar{\psi}}{\partial t} = -\frac{h}{4\pi i} \left(\nabla^2 - \frac{8\pi^2}{h^2} V \right) \bar{\psi}$$

are multiplied by $\rho \bar{\psi}$ and $\rho \psi$ respectively, and added. Hence

(39)
$$\frac{\partial}{\partial t}(\rho\psi\bar{\psi}) = \frac{h}{4\pi i}\rho \cdot (\bar{\psi}\nabla^2\psi - \psi\nabla^2\bar{\psi}).$$

To carry out in extenso the transformation of the right-hand side, we must remember the explicit form of our many-dimensional, non-Euclidean, Laplacian operator:

(40)
$$\rho \nabla^2 = \sum_{k} \frac{\partial}{\partial q_k} \left[\rho T_{p_k} \left(q_l, \frac{\partial \psi}{\partial q_l} \right) \right].$$

By a small transformation we readily obtain

(41)
$$\frac{\partial}{\partial t}(\rho\psi\bar{\psi}) = \frac{h}{4\pi i} \sum_{k} \frac{\partial}{\partial q_{k}} \left[\rho\bar{\psi}T_{p_{k}}\left(q_{l}, \frac{\partial\psi}{\partial q_{l}}\right) - \rho\psi T_{p_{k}}\left(q_{l}, \frac{\partial\bar{\psi}}{\partial q_{l}}\right) \right].$$

The right-hand side appears as the divergence of a many-dimensional real vector, which is evidently to be interpreted as the current density of the weight-function in configuration space. Equation (41) is the continuity equation of the weight-function.

From it we can obtain the equation of continuity of electricity, and, indeed, a separate equation of this sort is valid for the charge density "originating from each separate particle". Let us fix on the ath particle, say. Let its "charge" be e_a , its mass m_a , and let its coordinate space be described by Cartesians x_a , y_a , z_a , for the sake of simplicity. We denote the product of the differentials of the remaining co-ordinates shortly by dx. Over the latter, we integrate equation (41), keeping x_a , y_a , z_a , fixed. As the result, all terms except three disappear from the right-hand side, and we obtain

(42)
$$\begin{cases} \frac{\partial}{\partial t} \left[e_{\alpha} \int \psi \bar{\psi} dx' \right] = \frac{he_{\alpha}}{4\pi i m_{\alpha}} \left\{ \frac{\partial}{\partial x_{\alpha}} \left[\int \left(\bar{\psi} \frac{\partial \psi}{\partial x_{\alpha}} - \psi \frac{\partial \bar{\psi}}{\partial x_{\alpha}} \right) dx' \right] + \frac{\partial}{\partial y_{\alpha}} \left[\int \left(\bar{\psi} \frac{\partial \psi}{\partial y_{\alpha}} - \psi \frac{\partial \bar{\psi}}{\partial y_{\alpha}} \right) dx' \right] + \dots \right\} \\ = \frac{he_{\alpha}}{4\pi i m_{\alpha}} \operatorname{div}_{\alpha} \left[\int \left(\bar{\psi} \operatorname{grad}_{\alpha} \psi - \psi \operatorname{grad}_{\alpha} \bar{\psi} \right) dx' \right]. \end{cases}$$

In this equation, div and grad have the usual three-dimensional Euclidean meaning, and x_a , y_a , z_a are to be interpreted as Cartesian co-ordinates of real space. The equation is the continuity equation of that charge density which "originates from the ath particle". If we form all the others in an analogous fashion, and add them together, we obtain the total equation of continuity. Of course, we must emphasize that the interpretation of the integrals on the right-hand side as components of the current density, is, as in all such cases, not absolutely compulsory, because a divergence-free vector could be added thereto.

To give an example, in the conservative *one*-electron problem, if ψ is given by

¹ Cf. paper on Heisenberg's theory, equation (31). The quantity there denoted by $\Delta_x - \mathbf{i}$ is our "density function" $\rho(x)$ (e.g. $r^2 \sin \theta$ in spherical polars). T is the kinetic energy as function of the position co-ordinates and momenta, the suffix at T denoting differentiation with respect to a momentum. In equations (31) and (32), loc. cit., unfortunately by error the suffix k is used twice, once for the summation and then also as a representative suffix in the argument of the functions.

(43)
$$\psi = \sum_{k} c_k u_k e^{2\pi i \nu_k t + i\theta_k} \quad (c_k, \theta_k \text{ real constants}),$$

we get for the current density J

(44)
$$J = \frac{he_1}{2\pi m_1} \sum_{(k, l)} c_k c_l (u_l \operatorname{grad} u_k - u_k \operatorname{grad} u_l) \cdot \sin [2\pi (\nu_k - \nu_l)t + \theta_k - \theta_l].$$

We see, and this is valid for conservative systems generally, that, if only a single proper vibration is excited, the current components disappear and the distribution of electricity is constant in time. The latter is also immediately evident from the fact that $\psi\bar{\psi}$ becomes constant with respect to the time. This is still the case even when several proper vibrations are excited, if they all belong to the same proper value. On the other hand, the current density then no longer needs to vanish, but there may be present, and generally is, a stationary current distribution. Since the one or the other occurs in the unperturbed normal state at any rate, we may in a certain sense speak of a return to electrostatic and magnetostatic atomic models. In this way the lack of radiation in the normal state would, indeed, find a startingly simple explanation.

I hope and believe that the present statements will prove useful in the elucidation of the magnetic properties of atoms and molecules, and further for explaining the flow of electricity in solid bodies.

Meantime, there is no doubt a certain crudeness in the use of a complex wave function. If it were unavoidable in principle, and not merely a facilitation of the calculation, this would mean that there are in principle two wave functions, which must be used together in order to obtain information on the state of the system. This somewhat unacceptable inference admits, I believe, of the very much more congenial interpretation that the state of the system is given by a real function and its time-derivative. Our inability to give more accurate information about this is intimately connected with the fact that, in the pair of equations (4"), we have before us only the substitute—extraordinarily convenient for the calculation, to be sure—for a real wave equation of probably the fourth order, which, however, I have not succeeded in forming for the non-conservative case.

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