"Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen," Zeit. Phys. 33 (1925), 879-893.

# On the quantum-theoretical reinterpretation of kinematical and mechanical relationships

By W. Heisenberg in Göttingen

(Received on 29 July 1925)

Translated by D. H. Delphenich

In this paper, we will attempt to achieve a quantum-theoretical mechanics that is based exclusively upon relationships between quantities that are observable, in principle.

It is known that one can raise the serious objection to the formal rules that are generally employed in quantum theory for the calculation of observable quantities (e.g., energy in the hydrogen atom) that those rules of calculation are obtained essentially as constituent relations between quantities that cannot be observed, in principle (such as, e.g., the position or orbital period of the electron), so those rules will obviously lack any intuitive physical foundation if one would not like to continue to maintain the hope that those up-to-now unobservable quantities might perhaps be made experimentally accessible at some later point. That hope could be regarded as justified if the stated rules were applied to a certain unlimited domain of quantum-theoretical problems in an intrinsically consistent way. However, experiment shows that only the hydrogen atom and the Stark effect of that atom obey those formal rules of quantum theory, but that fundamental difficulties will appear already in the problem of "crossed fields" (e.g., the hydrogen atom in electric and magnetic fields of different directions), namely, that the reaction of the atom to periodically-varying fields certainly cannot be described by the stated rules and that ultimately an extension of the quantum rules to the treatment of the atom and many atoms has proven to be impossible. It was customary to refer to this breakdown of the quantum-theoretical rules, which can indeed be characterized essentially by applying classical mechanics, as a deviation from classical mechanics. However, that relationship can hardly be regarded as an analogy when one considers that already the **Einstein-Bohr** frequency condition (which is indeed valid in full generality) represents such a complete negation of classical mechanics, or even better, from the standpoint of wave theory, of the kinematics that this mechanics is based upon, that one cannot think of there being an absolute validity of classical mechanics even for the simplest quantum-theoretical problems. From this state of affairs, it seems more advisable to give up completely on any hope of an observation of the hithertounobservable quantities (such as the position and orbital period of the electron), and thus, at the same time, to grant that the partial agreement between the stated quantum rules and experiment is more-or-less coincidental and to attempt to construct a quantum-theoretical mechanics that would be analogous to classical mechanics in which only relations between observable quantities would be present. One can regard not only the frequency condition, but also **Kramer**'s dispersion theory  $(^1)$  and the further work that was done on that theory  $(^2)$  as the most important initial Ansätze for such a quantum-theoretical mechanics. In what follows, we would like to seek to present some new quantum-mechanical relations and to employ them for a complete treatment of some special problems. Therefore, we will restrict ourselves to problems of one degree of freedom.

§ 1. – In the classical theory, the radiation of a moving electron (in the wave zone – i.e.,  $\mathfrak{E} \sim \mathfrak{H} \sim 1 / r$ ) is given by not just the expressions:

$$\mathfrak{E} = \frac{e}{r^3 c^2} [\mathfrak{r}[\mathfrak{r}\dot{\mathfrak{v}}]],$$
$$\mathfrak{H} = \frac{e}{r^2 c^2} [\dot{\mathfrak{v}}\mathfrak{r}],$$

but also some terms that one must add in the next approximation -e.g., ones of the form:

$$\frac{e}{rc^3}\dot{\mathfrak{v}}\mathfrak{v},$$

which one can refer to as "quadrupole radiation," and terms of even higher approximations -e.g., ones of the form:

$$\frac{e}{rc^4}\dot{\mathfrak{v}}\mathfrak{v}^2$$

The approximation can be continued arbitrarily far in this way. (In the foregoing  $\mathfrak{E}$ ,  $\mathfrak{H}$  mean the field strengths at the reference point, *e* means the charge of the electron,  $\mathfrak{t}$  means the distance from the electron to the reference point, and  $\mathfrak{v}$  means the velocity of the electron).

One can ask what those higher terms must look like in quantum theory. Since the higher approximations can be calculated simply in the classical theory when the motion of the electron (its Fourier representation, resp.) is given, one would expect something similar to be true in quantum theory. That question has nothing to do with electrodynamics, but it has a purely *kinematical* nature, and that seems especially important to us. We can pose it in its simplest form as follows: If one is given quantum-theoretical quantity that enters in place of the classical quantity x(t) then what quantum-theoretical quantity would enter in place of  $x(t)^2$ ?

<sup>(&</sup>lt;sup>1</sup>) **H. A. Kramers**, Nature **113** (1924), 673.

<sup>(&</sup>lt;sup>2</sup>) M. Born, Zeit. Phys. 26 (1924), 379. H. A. Kramers and W. Heisenberg, Zeit. Phys. 31 (1925),

<sup>681.</sup> M. Born and P. Jordan, Zeit. Phys. (to appear).

Before we can answer that question, we must recall that in quantum theory it is not possible to assign a point in space that is a function of time to an electron by means of observable quantities. But the electron can probably be also assigned radiation in the quantum theory. That radiation will be described, first of all, by the frequencies that appear as functions of two variables, which take the form:

$$V(n, n - \alpha) = \{W(n) - W(n - \alpha)\}$$

in quantum theory and the form:

$$v(n, \alpha) = \alpha \cdot v(n) = \alpha \frac{1}{h} \frac{dW}{dn}$$

in classical theory. (In this,  $n \cdot h = J$ , which is one of the canonical constants.)

One can write down the following combining relations as characteristic of the comparison between classical and quantum theory in regard to the frequencies:

#### <u>Classical</u>

$$V(n, \alpha) + V(n, \beta) = V(n, \alpha + \beta).$$

# Quantum-theoretical

$$v(n, n-\alpha) + v(n-\alpha, n-\alpha-\beta) = v(n, n-\alpha-\beta)$$

or

$$V(n-\beta, n-\alpha-\beta) + V(n, n-\beta) = V(n, n-\alpha-\beta),$$

resp.

Along with the frequencies, the amplitudes are necessary for the description of radiation; the amplitudes can be regarded as complex vectors (with six independent determining data), and they determine polarization and phase. They are also functions of the two variables n and a, such that part of the radiation in question can be represented by the following expression:

# Quantum-theoretical

$$\operatorname{Re}\left\{\mathfrak{A}\left(n,n-\alpha\right)e^{i\,\omega\left(n,\,n-\alpha\right)\,t}\right\}$$
(1)

#### <u>Classical</u>

$$\operatorname{Re}\left\{\mathfrak{A}_{\alpha}(n) e^{i \,\omega(n) \cdot \,\alpha t}\right\}$$
(2)

The phase (which is included in  $\mathfrak{A}$ ) does not seem to have a physical meaning in quantum theory at first, since the frequencies of quantum theory are not commensurable with higher harmonics, in general. However, we will see immediately that the phase also have a well-defined meaning in quantum theory that is analogous to the one that it has in

classical theory. If we now consider a well-defined quantity x(t) in the classical theory then we can think of it as being represented by a set of quantities of the form:

$$\mathfrak{A}_{\alpha}(n) e^{i \, \omega(n) \cdot \, \alpha t},$$

which can be combined into a sum or integral x(t) that is represented by:

$$x(n,t) = \sum_{\alpha = -\infty}^{+\infty} \mathfrak{A}_{\alpha}(n) e^{i\omega(n) \cdot \alpha t},$$
  
or  
$$x(n,t) = \int_{-\infty}^{+\infty} \mathfrak{A}_{\alpha}(n) e^{i\omega(n) \cdot \alpha t} d\alpha,$$
  
resp. (2a)

Due to the equal status of the quantities  $n, n - \alpha$ , such a combination of the corresponding quantum-theoretical quantities does not seem possible without some arbitrariness, and for that reason, it is not reasonable. However, one can probably regard the set of quantities:

$$\mathfrak{A}_{\alpha}(n, n-\alpha) e^{i \omega(n, n-\alpha) t}$$

as the representative of the quantities x(t) and then look for the answer to the question that was posed above: How will the quantity  $x(t)^2$  be represented?

Obviously the answer reads:

$$\mathfrak{B}_{\alpha}(n) e^{i \,\omega(n)\,\beta t} = \sum_{\alpha=-\infty}^{+\infty} \mathfrak{A}_{\alpha} \,\mathfrak{A}_{\beta-\alpha} e^{i\omega(n)(\alpha+\beta-\alpha)t}$$
(3)

or

$$=\int_{-\infty}^{+\infty}\mathfrak{A}_{\alpha}\,\mathfrak{A}_{\beta-\alpha}\,e^{i\,\omega(n)(\alpha+\beta-\alpha)t}d\alpha\,,\tag{4}$$

resp., classically, in which one then has:

$$x(t)^{2} = \sum_{\beta = -\infty}^{+\infty} \mathfrak{B}_{\beta}(n) e^{i\omega(n)\beta t}$$
(5)

or

$$= \int_{-\infty}^{+\infty} \mathfrak{B}_{\beta}(n) e^{i\omega(n)\beta t} d\beta, \qquad (6)$$

resp.

Quantum-theoretically, the simplest and most natural assumption seems to be to replace the relations (3, 4) with the following ones:

$$\mathfrak{B}_{\alpha}(n,n-\beta) e^{i\,\omega(n,n-\beta)\,t} = \sum_{\alpha=-\infty}^{+\infty} \mathfrak{A}(n,n-\alpha)\,\mathfrak{A}(n-\alpha,n-\beta)\,e^{i\,\omega(n,n-\beta)\,t} \tag{7}$$

or

$$= \int_{-\infty}^{+\infty} d\alpha \mathfrak{A}(n, n-\alpha) \mathfrak{A}(n-\alpha, n-\beta) e^{i\omega(n, n-\beta)t}, \qquad (8)$$

resp., and indeed this type of combination will be implied almost inevitably by the combining relations of the frequencies. If one makes the assumptions (7) and (8) then one will also recognize that the phases of the quantum-theoretical  $\mathfrak{A}$  have just a great a physical meaning as the ones in the classical theory, only the starting point in time, and therefore a phase constant that would be *common* to all  $\mathfrak{A}$ , is arbitrary and physically meaningless. However, the phases of the *individual*  $\mathfrak{A}$  enter essentially into the quantity  $\mathfrak{B}$  (<sup>1</sup>). A geometric interpretation of such quantum-theoretical phase relationships in analogy with then ones in the classical theory seems hardly possible.

If we further ask what the representative of the quantity  $x(t)^3$  would be then we would find with no difficulty:

# <u>Classically</u>

$$\mathfrak{C}(n,\gamma) = \sum_{\alpha=-\infty}^{+\infty} \sum_{\beta=-\infty}^{+\infty} \mathfrak{A}_{\alpha}(n) \mathfrak{A}_{\beta}(n) \mathfrak{A}_{\gamma-\alpha-\beta}(n)$$
(9)

#### Quantum-theoretically

$$\mathfrak{C}(n, n-\gamma) = \sum_{\alpha=-\infty}^{+\infty} \sum_{\beta=-\infty}^{+\infty} \mathfrak{A}_{\alpha}(n, n-\alpha) \mathfrak{A}_{\beta}(n-\alpha, n-\alpha-\beta) \mathfrak{A}_{\gamma-\alpha-\beta}(n-\alpha-\beta, n-\gamma) , \quad (10)$$

or the corresponding integrals, resp.

All quantities of the form  $x(t)^n$  can be represented quantum-theoretically in a similar way, and when any function is given f[x(t)], one can obviously always find the quantum-theoretical analogue when that function can be developed in power series in x. However, an essential difficulty will arise when we consider *two* quantities x(t), y(t) and ask what the product x(t) y(t) would be.

Let x(t) be characterized by  $\mathfrak{A}$  and y(t) be characterized by  $\mathfrak{B}$ , so the representation of x(t) y(t) would be:

Classically

$$\mathfrak{C}_{\beta}(n) = \sum_{\alpha = -\infty}^{+\infty} \mathfrak{A}_{\alpha}(n) \mathfrak{B}_{\beta - \alpha}(n)$$

<sup>(&</sup>lt;sup>1</sup>) Cf., also **H. A. Kramers** and **W. Heisenberg**, *loc. cit.* The phases enter into the expressions for the induced scattering momentum in that article in an essential way.

$$\mathfrak{C}(n, n-\beta) = \sum_{\alpha=-\infty}^{+\infty} \mathfrak{A}_{\alpha}(n, n-\alpha) \mathfrak{B}(n-\alpha, n-\beta)$$

Whereas classically x(t) y(t) is always equal to y(t) x(t), this does not need to be the case in quantum theory, in general. In special cases – e.g., when one forms  $x(t) \cdot x(t)^2$  – this difficulty will not arise.

If one is dealing with expressions of the form:

$$v(t)\dot{v}(t)$$
,

as in the question that was posed at the beginning of that paragraph, then one should replace  $v\dot{v}$  with  $(v\dot{v}+\dot{v}v)/2$  quantum-theoretically, in order to succeed in making  $v\dot{v}$  appear as the differential quotient of  $v^2/2$ . In a similar way, one can probably always give quantum-mechanical mean values in a natural way, which will generally be hypothetical to a higher degree than formulas (7) and (8).

Apart from the difficulty that was just described, formulas of type (7), (8) must generally be satisfied in order for one to also express the interaction of electrons in an atom in terms of the characteristic amplitudes of the electrons.

§ 2. – With these arguments, which have the kinematics of quantum theory as their subject, we now go on to the mechanical problems, which are directed towards the determination of  $\mathfrak{A}$ ,  $\nu$ , W from the given forces of the system. In the theory up to now, that problem is solved in two steps:

1. Integrate the equation of motion:

$$\ddot{x} + f(x) = 0.$$
 (11)

2. Determine the constant for periodic motion from:

$$\oint p \, dq = \oint m \, \dot{x} \, dx = J \, (= nh). \tag{12}$$

When one sets out to construct a quantum-theoretical theory of mechanics that is as analogous as possible to the classical one, it would probably be reasonable to adapt the equation of motion (11) to the quantum theory directly, in which it would only be necessary – in order to not depart from certain fundamental facts about quantities that are unobservable, in principle – to replace the quantities  $\ddot{x}$ , f(x) with their quantum-theoretical representatives. In the classical theory, it is possible to look for the solution of (11) by the Ansatz of expanding x into a Fourier series (Fourier integral, resp.) with undetermined coefficients (and frequencies). We will generally obtain infinitely-many equations in infinitely-many unknowns (integral equations, resp.) that can be converted

into recursion formulas for the  $\mathfrak{A}$  only in special cases. However, in quantum theory, we are tentatively dependent upon this kind of solution to (11), since, as we discussed above, none of the functions x (n, f) can be defined to be an analogous quantum-theoretical function.

This has the consequence that the quantum-theoretical solution of (11) can be carried out only in the simplest cases, at first. Before we go into those simple examples, let us derive the quantum-theoretical determination of the constant from (12). We thus assume that the (classical) motion is periodic:

$$x = \sum_{\alpha = -\infty}^{+\infty} a_{\alpha}(n) e^{i \, a \, \omega_n t} \, ; \tag{13}$$

one then has:

$$m\dot{x} = m\sum_{\alpha=-\infty}^{+\infty} a_{\alpha}(n) \cdot i\alpha \,\omega_n \,e^{i\,a\omega_n t}$$

and

$$\oint m \dot{x} dx = \oint m \dot{x}^2 dt = 2\pi m \sum_{\alpha = -\infty}^{+\infty} a_{\alpha}(n) a_{-\alpha}(n) \alpha^2 \omega_n$$

Since one further has  $a_{-\alpha}(n) = \overline{a_{\alpha}(n)}$  (x shall be real), it will follow that:

$$\oint m \dot{x}^2 dt = 2\pi m \sum_{\alpha = -\infty}^{+\infty} |a_{\alpha}(n)|^2 \alpha^2 \omega_n .$$
(14)

Up to now, one mostly sets that phase integral is equal to a whole number multiple of h, and thus to  $n \cdot h$ . However, such a condition is not only very constraining of the mechanical calculation, it also seems arbitrary, in the sense of the correspondence principle, from the standpoint that has been taken up to now. Analogously, the J are only established up to an additive constant as whole-number multiples of h, and in place of (14), one will naturally find:

 $\frac{d}{dn}(n h) = \frac{d}{dn} \cdot \oint m \dot{x}^2 dt ;$ 

that is:

$$h = 2\pi m \cdot \sum_{\alpha = -\infty}^{+\infty} \alpha \frac{d}{dn} (\alpha \omega_n \cdot |a_{\alpha}|^2).$$
(15)

Such a condition generally establishes the  $a_{\alpha}$  also only up to a constant, and empirically this indeterminacy will give rise to difficulties in the appearance of half-integer quantum numbers.

If we ask whether there is a quantum-theoretical relation between observable quantities that corresponds to (14) and (15) then that will once more restore the missing uniqueness in its own right.

Indeed, it is only equation (15) that possesses a simple quantum-theoretical conversion  $(^{1})$  that is connected with **Kramer**'s dispersion theory:

$$h = 4\pi m \sum_{\alpha=0}^{\infty} \{ |a(n, n+\alpha)|^2 \omega(n, n+\alpha) - |a(n, n-\alpha)|^2 \omega(n, n-\alpha) \},$$
(16)

but this relation suffices to determine the *a* uniquely here, anyway. The initiallyundetermined constant in the quantities *a* will be established in its own right by the condition that there should be a normal state from which no more radiation can take place. Let the normal state be denoted by  $n_0$ , such that:

$$a(n_0, n_0 - \alpha) = 0$$
 (for all  $\alpha > 0$ ).

The question of half-integer or integer quantization should therefore not arise in a quantum theory of mechanics that employs only relations between observable quantities.

Equations (11) and (16) together, when they can be solved, contain a complete determination of not only the frequencies and energies, but also the quantum-theoretical transition probabilities. However, the actual mathematical implementation of that can be achieved only in the simplest cases, for now. A special complication also arises for many systems (such as, e.g., hydrogen atoms) in such a way that some of the solutions will correspond to periodic motions, while others will correspond to aperiodic ones, which has the consequence that the quantum-theoretical series (7), (8), and equation (16) will always split into a sum and an integral. Quantum-mechanically, a split into "periodic and aperiodic motions" cannot generally be performed.

Nonetheless, one can perhaps regard equations (11) and (16), at least, in principle, as a satisfactory solution of the mechanical problem when one can show that this solution coincides with (does not contradict, resp.) the quantum-theoretical relationships that are known up to now, and therefore that a small perturbation of a mechanical problem will give rise to additional terms in the energies (frequencies, resp.) that correspond to just the expressions that **Kramers** and **Born** found, in contrast to the ones that the classical theory would deliver. One must further examine whether, in general, equation (11) also corresponds to an energy integral  $\frac{1}{2}m\dot{x}^2 + U(x) = \text{const.}$  in the quantum-theoretical picture that is proposed here and whether the energy thus-obtained (similarly to what is true classically  $v = \partial W / \partial J$ ) satisfies the condition  $\Delta W = h \cdot v$ . A general response to that question could first exhibit the intrinsic connection between the quantum-mechanical attempts up to now and lead to quantum mechanics that consequently only operated with observable quantities. Except for a general relation between **Kramer's** dispersion formulas and equations (11) and (16), we can answer the questions that were posed above only in the entirely specialized cases that can be solved by a simple recursion.

That general relationship between **Kramer**'s dispersion theory and our equations (11), (16) consists of the fact that it follows from equation (11) (i.e., its quantum-theoretical analogue), just as it does in the classical theory, that the oscillating electron behaves like a free electron compared to light, which has much shorter wave lengths than

<sup>(&</sup>lt;sup>1</sup>) This relation was given already on the basis of the consideration of dispersion by **W. Kuhn**, Zeit. Phys. **33** (1925), 408, and **Thomas**, Naturwiss. **13** (1925).

all of the eigen-oscillations of the system. That result also follows from **Kramers**'s theory when one considers equation (16). In fact, **Kramers** found that the moment that is induced by the wave  $E \cos 2\pi v t$ :

$$M = e^{2} E \cos 2\pi v t \cdot \frac{2}{h} \sum_{\alpha=0}^{\infty} \left\{ \frac{|a(n, n+\alpha)|^{2} v(n, n+\alpha)}{v^{2}(n, n+\alpha) - v^{2}} - \frac{|a(n, n+\alpha)|^{2} v(n, n-\alpha)}{v^{2}(n, n-\alpha) - v^{2}} \right\},$$

and thus for  $v \gg v(n, n + a)$ :

$$M = -\frac{2Ee^{2}\cos 2\pi vt}{v^{2} \cdot h} \sum_{\alpha=0}^{\infty} \{ |a(n, n+\alpha)|^{2} v(n, n+\alpha) - |a(n, n-\alpha)|^{2} v(n, n-\alpha) \},\$$

which goes to:

$$M = -\frac{e^2 E \cos 2\pi v t}{v^2 \cdot 4\pi^2 m},$$

due to (16).

§ 3. – As the simplest example, we shall treat the anharmonic oscillator in what follows:

$$\ddot{x} + \omega_0^2 x + \lambda x^2 = 0. \tag{17}$$

Classically, this equation can be satisfied by an Ansatz of the form:

$$x = \lambda a_0 + a_1 \cos \omega t + \lambda a_0 \cos 2\omega t + \lambda^2 a_3 \cos 3\omega t + \ldots + \lambda \tau^{-1} a_\tau \cos \tau \omega t,$$

in which the *a* are power series in  $\lambda$  that begin with terms that are free of  $\lambda$ . We shall attempt to make an analogous quantum-theoretical Ansatz and represent *x* by terms of the form:

$$\lambda a(n, n), \qquad a(n, n-1)\cos \omega(n, n-1)t, \qquad \lambda a(n, n-2)\cos \omega(n, n-2)t,$$
$$\dots, \lambda^{\tau-1} a(n, n-1)\cos \omega(n, n-1)t, \dots$$

From equations (3), (4) [(7), (8), resp.], the recursion formulas for the determination of the *a* and  $\omega(\text{up to terms of order } \lambda)$  read:

# Classically

$$\omega_{0}^{2} a_{0}(n) + \frac{a_{1}^{2}(n)}{2} = 0, -\omega^{2} + \omega_{0}^{2} = 0, (-4\omega^{2} + \omega_{0}^{2}) a_{2}(n) + \frac{a_{1}^{2}(n)}{2} = 0, (-9\omega^{2} + \omega_{0}^{2}) a_{3}(n) + a_{1} a_{2} = 0, \dots$$
(18)

# Quantum-theoretically

$$\omega_{0}^{2} a_{0}(n) + \frac{a^{2}(n+1,n) + a^{2}(n,n-1)}{2} = 0,$$
  

$$-\omega^{2}(n,n-1) + \omega_{0}^{2} = 0,$$
  

$$(-\omega^{2}(n,n-2) + \omega_{0}^{2}) a(n,n-2) + \frac{a(n,n-1)a(n-1,n-2)}{2} = 0,$$
  

$$(-\omega^{2}(n,n-3) + \omega_{0}^{2}) a(n,n-3) + \frac{a(n,n-1)a(n-1,n-3)}{2} + \frac{a(n,n-2)a(n-2,n-3)}{2} = 0,$$
  
.....

The quantum condition:

Classical 
$$(J = nh)$$

$$1 = 2\pi m \frac{d}{dJ} \sum_{\tau=-\infty}^{+\infty} \tau^2 \frac{|a_{\tau}|^2 \omega}{4}$$

# Quantum-theoretically

$$h = \pi m \sum_{\tau=0}^{\infty} \left[ |a(n+\tau, n)|^2 \omega(n+\tau, n) - |a(n, n-\tau)|^2 \omega(n, n-\tau) \right]$$

must be added to this.

In the first approximation, this implies that:

$$a_1^2(n), \qquad a^2(n, n-1), \text{ resp.}, = \frac{(n+\text{const})h}{\pi m \omega_0},$$
 (20)

classically, as well as quantum-theoretically.

Quantum-theoretically, the constant in (20) can be determined in such a way that  $a(n_0, n_0 - 1)$  should be zero in the normal state. If we number the *n* in such a way that *n* equals zero in the normal state – so  $n_0 = 0$  – then it will follow that:

$$a^2(n,n-1)=\frac{nh}{\pi m\,\omega_0}$$

It then follows from the recursion equations (18) that in the classical theory  $a_{\tau}$  (in the first approximation in  $\lambda$ ) will have the form  $\kappa(\tau) n^{\tau/2}$ , where  $\kappa(\tau)$  represents a factor that is independent of *n*. In quantum theory, (19) implies that:

$$a(n, n-\tau) = \kappa(\tau) \sqrt{\frac{n!}{(n-\tau)!}}, \qquad (21)$$

in which  $\kappa$  ( $\tau$ ) represents the same proportionality factor that is independent of n. Naturally, for large values of n, the quantum-theoretical value of  $a_{\tau}$  will go to the classical one asymptotically.

For the energy, it is reasonable to try the classical Ansatz:

$$\frac{m\,\dot{x}^2}{2} + m\,\omega_0^2\,\frac{x^2}{2} + \frac{m\lambda}{3}\,x^3 = W_1$$

which is also actually quantum-theoretically constant in the approximation that we are calculating in here, and from (19), (20), (21), it will have the value:

# Classically

$$W = \frac{n h \omega_0}{2\pi} \tag{22}$$

# Quantum-theoretical [from (7), (8)]

$$W = \frac{(n + \frac{1}{2})h\,\omega_0}{2\pi}$$
(23)

(up to quantities of order  $\lambda^2$ ).

In this picture, the energy cannot be represented by "classical mechanics" [i.e., (22)], even for the harmonic oscillator, but it will have the form (23).

The more precise calculation in the higher approximation in W, a,  $\omega$  shall also be carried out in the simplest example of the anharmonic oscillator of the type:

$$\ddot{x} + \omega_0^2 x + \lambda x^3 = 0.$$

Classically, one can set:

$$x = a_1 \cos \omega t + \lambda a_3 \cos 2\omega t + \lambda^3 a_5 \cos 5\omega t + \dots$$

here, and analogously, one can try the quantum-mechanical Ansatz:

$$a(n, n-1)\cos \omega(n, n-1)t,$$
  $\lambda a(n, n-3)\cos \omega(n, n-3)t,$  ...

The quantities a are once more power series in  $\lambda$  whose first terms have the form:

$$a(n, n-\tau) = \kappa(\tau) \sqrt{\frac{n!}{(n-\tau)!}},$$

as in (21), which one will obtain by calculating the equations that correspond to equations (18), (19).

If one performs the calculation of  $\omega$ , *a* from (18), (19) up to the approximation  $\lambda^2$  ( $\lambda$ , resp.) then one will get:

$$\omega(n, n-1) = \omega_0 + \lambda \cdot \frac{2nh}{8\pi \,\omega_0^2 \,m} - \lambda^2 \cdot \frac{3h^2}{256 \,\omega_0^5 \,m^2 \pi^2} \,(17n^2 + 7) + \dots, \tag{24}$$

$$a(n, n-1) = \sqrt{\frac{nh}{\pi \,\omega_0 \,m}} \left( 1 - \lambda \frac{3nh}{16\pi \,\omega_0^3 \,m} + \cdots \right) - \lambda^2 \cdot \frac{3h^2}{256 \,\omega_0^5 \,m^2 \pi^2} \,, \tag{25}$$

$$a(n, n-3) = \frac{1}{32} \sqrt{\frac{h^3}{\pi^3 \,\omega_0^7 \,m^3} n(n-1)(n-2)} \left( 1 - \lambda \frac{39(n-1)h}{32\pi \,\omega_0^3 \,m} + \cdots \right).$$
(26)

The energy, which is defined to be the constant term in:

$$m\frac{\dot{x}^2}{2} + m\omega_0^2 \frac{x^2}{2} + \frac{m\lambda}{4}x^4$$

(I cannot generally prove that the periodic terms are actually all zero, but that was true for the terms that I calculated), yields:

$$W = \frac{(n+\frac{1}{2})h\omega_0}{2\pi} + \lambda \cdot \frac{3(n^2+n+\frac{1}{2})h^2}{8\cdot 4\pi^2\omega_0^2 \cdot m} - \lambda^2 \cdot \frac{h^3}{512\pi^3\omega_0^5 m^2} \left(17n^3 + \frac{51}{2}n^2 + \frac{59}{2}n + \frac{21}{2}\right).$$
(27)

One can also calculate this energy from the **Kramers-Born** procedure when one regards the term  $(m\lambda / 4) x^4$  as a perturbation terms to the harmonic oscillator. One actually comes once more to the precisely the result (27), which seems to be to be a remarkable vote of confidence for the basic equations of quantum mechanics. Furthermore, the energy that is calculated from (27) fulfills the formula [cf., (24)]:

$$\frac{\omega(n,n-1)}{2\pi} = \frac{1}{h} \cdot [W(n) - W(n-1)],$$

which is likewise to be considered as the necessary condition for the possibility of determining the corresponding transition probabilities from one of equations (11) and (16).

In conclusion, let us cite the rotator as an example and refer to the relationship between equations (7), (8) and the intensity formulas for the Zeeman effect  $(^1)$  and for multiplets  $(^2)$ .

Let the rotator be represented by an electron that orbits around a nucleus at a *constant* distance. The "equations of motion" then say (classically, as well as quantum-theoretically) only that the electron at a constant distance a describes a uniform planar rotation around the nucleus with the angular velocity  $\omega$ . From (12), the "quantum condition" (16) implies that:

$$h = \frac{d}{dn} (2\pi m a^2 \omega),$$

and from (16):

$$h = 2\pi m \{a^2 \ \omega(n+1, n) - a^2 \ \omega(n, n-1)\}$$

from which it will follow, in both cases, that:

$$\omega(n, n-1) = \frac{h \cdot (n + \text{const.})}{2\pi m a^2}$$

The condition that the radiation should vanish in the normal state ( $n_0 = 0$ ) leads to the formula:

$$\omega(n, n-1) = \frac{h \cdot n}{2\pi m a^2}.$$
(28)

The energy will be:

$$W=\frac{m}{2}v^2,$$

or, from (7), (8):

$$W = \frac{m}{2}a^2 \cdot \frac{\omega^2(n, n-1) + \omega^2(n+1, n)}{2} = \frac{h^2}{8\pi^2 m a^2} (n^2 + n + \frac{1}{2}), \qquad (29)$$

which again satisfies the condition that  $\omega(n, n-1) = \frac{2\pi}{h} [W(n) - W(n-1)]$ . As support

for the formulas (28) and (29), which deviate from the usual theory up to now, one can consider that according to **Kratzer** ( $^3$ ), many band spectra (also ones for which the existence of an electron impulse is improbable) seem to demand formulas of type (28), (29) (which one has sought to explain in the classical-mechanical theory by the use of half-integer quantization, up to now).

<sup>(&</sup>lt;sup>1</sup>) Goudsmit and R. de L. Kronig, Naturwiss. 13 (1925), 90; H. Hönl, Zeit. Phys. 31 (1925), 340.

<sup>(&</sup>lt;sup>2</sup>) **R. de L. Kronig**, Zeit. Phys. **31**(1925), 885; **A. Sommerfeld** and **H. Hönl**, Sitzber. d. Preuss. Akad. (1925), 141; **H. N. Russell**, Nature **115** (1925), 835.

<sup>(&</sup>lt;sup>3</sup>) Cf., e.g., **B. A. Kratzer**, Sitzber. d. Bayr. Akad. (1922), 107.

In order to arrive at the **Goudsmit-Kronig-Hönl** formulas, we must leave the domain of the problem with one degree of freedom and assume that the rotator, which has any direction in space, performs a very slow precession v around the *z*-axis of an external field. The quantum number that corresponds to that precession will be called *m*. The motion will then be represented by the quantities:

$$z: a (n, n-1; m, m) \cos \omega(n, n-1) t, x + iy: b (n, n-1; m, m-1) e^{i [\omega(n, n-1) + v] t}, b (n, n-1; m-1, m) e^{i [-\omega(n, n-1) + v] t}.$$

The equations of motion read simply:

$$x^2 + y^2 + z^2 = a^2,$$

which, from (7), gives rise to the equations  $(^1)$ :

$$\frac{1}{2}\left\{\frac{1}{2}a^{2}(n, n-1; m, m) + b^{2}(n, n-1; m, m-1) + b^{2}(n, n-1; m, m+1) + \frac{1}{2}a^{2}(n+1, n; m, m) + b^{2}(n-1, n; m-1, m) + b^{2}(n+1, n; m+1, m)\right\} = a^{2},$$
(30)

$$\frac{1}{2}a(n, n-1; m, m) a(n-1, n-2; m, m)$$
  
= b(n, n-1; m, m+1) b(n-1, n-2; m+1, m)  
+ b(n, n-1; m, m-1) b(n-1, n-2; m-1, m). (31)

From (16), the quantum condition:

$$2\pi m \{b^2(n, n-1; m, m-1) \ \omega(n, n-1) - b^2(n, n-1; m-1, m) \ \omega(n, n-1)\} = (m + \text{const}) \ h$$
(32)

must be added to this.

The classical relations that correspond to these equations:

$$\frac{\frac{1}{2}a_{0}^{2} + b_{1}^{2} + b_{-1}^{2} = a^{2}, \\ \frac{\frac{1}{2}a_{0}^{2} = b_{1}b_{-1}, \\ 2\pi m(b_{+1}^{2} - b_{-1}^{2}) = (m + \text{const})h \end{cases}$$
(33)

suffice to establish the *a*,  $b_1$ ,  $b_{-1}$  uniquely (up to the undetermined constant next to *m*).

The simplest solution of the quantum-theoretical equations (30), (31), (32) that one can offer reads:

$$b(n, n-1; m, m-1) = a \sqrt{\frac{(n+m+1)(n+m)}{4(n+\frac{1}{2})n}},$$

<sup>(&</sup>lt;sup>1</sup>) Equation (30) is essentially identical to the **Ornstein-Burger** sum rules.

$$b(n, n-1; m-1, m) = a \sqrt{\frac{(n-m)(n-m+1)}{4(n+\frac{1}{2})n}},$$
  
$$b(n, n-1; m, m-1) = a \sqrt{\frac{(n+m+1)(n+m)}{4(n+\frac{1}{2})n}},$$
  
$$a(n, n-1; m, m) = a \sqrt{\frac{(n+m+1)(n-m)}{(n+\frac{1}{2})n}}.$$

These expressions agree with the formulas of **Goudsmit**, **Kronig**, and **Hönl**. However, one not simply accept that these expressions represent the *only* solution of (30), (31), (32) – which seems to be likely when one observes the boundary conditions (viz., the vanishing of a, b on the "boundary"; cf., the cited papers of **Kronig**, **Sommerfeld**, and **Hönl**, **Russell**).

An argument that is similar to the one that was presented here will also lead from the intensity formulas for the multiplets to the result that the stated intensity rules are consistent with equations (7) and (16). This result, in turn, can serve to support the validity of the kinematic equation (7).

Whether a method for the determination of quantum-theoretical data from relations between observable quantities like the one that was proposed here can already be regarded as satisfactory, in principle, or whether that method represents only one more much-too-bold attack on the problem of formulating a quantum-theoretical mechanics (which is clearly quite physically difficult, from the outset) will first be clarified by a deeper mathematical examination of the method that was employed very superficially here.

Göttingen, Institut für theoretische Physik