

QUANTUM-THEORETICAL RE-INTERPRETATION OF KINEMATIC AND MECHANICAL RELATIONS

W. HEISENBERG

The present paper seeks to establish a basis for theoretical quantum mechanics founded exclusively upon relationships between quantities which in principle are observable.

It is well known that the formal rules which are used in quantum theory for calculating observable quantities such as the energy of the hydrogen atom may be seriously criticized on the grounds that they contain, as basic element, relationships between quantities that are apparently unobservable in principle, e.g., position and period of revolution of the electron. Thus these rules lack an evident physical foundation, unless one still wants to retain the hope that the hitherto unobservable quantities may later come within the realm of experimental determination. This hope might be regarded as justified if the above-mentioned rules were internally consistent and applicable to a clearly defined range of quantum mechanical problems. Experience however shows that only the hydrogen atom and its Stark effect are amenable to treatment by these formal rules of quantum theory. Fundamental difficulties already arise in the problem of 'crossed fields' (hydrogen atom in electric and magnetic fields of differing directions). Also, the reaction of atoms to periodically varying fields cannot be described by these rules. Finally, the extension of the quantum rules to the treatment of atoms having several electrons has proved unfeasible.

It has become the practice to characterize this failure of the quantum-theoretical rules as a deviation from classical mechanics, since the rules themselves were essentially derived from classical mechanics. This characterization has, however, little meaning when one realizes

Editor's note. This paper was published as Zs. Phys. 33 (1925) 879–893. It was signed 'Göttingen, Institut für theoretische Physik'.

that the *Einstein-Bohr* frequency condition (which is valid in all cases) already represents such a complete departure from classical mechanics, or rather (using the viewpoint of wave theory) from the kinematics underlying this mechanics, that even for the simplest quantum-theoretical problems the validity of classical mechanics simply cannot be maintained. In this situation it seems sensible to discard all hope of observing hitherto unobservable quantities, such as the position and period of the electron, and to concede that the partial agreement of the quantum rules with experience is more or less fortuitous. Instead it seems more reasonable to try to establish a theoretical quantum mechanics, analogous to classical mechanics, but in which only relations between observable quantities occur. One can regard the frequency condition and the dispersion theory of *Kramers*¹ together with its extensions in recent papers² as the most important first steps toward such a quantum-theoretical mechanics. In this paper, we shall seek to establish some new quantum-mechanical relations and apply these to the detailed treatment of a few special problems. We shall restrict ourselves to problems involving one degree of freedom.

1. In classical theory, the radiation emitted by a moving electron (in the wave zone, i.e., in the region where \mathfrak{E} and \mathfrak{H} are of the same order of magnitude as $1/r$) is not entirely determined by the expressions

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

but additional terms occur in the next order of approximation, e.g. terms of the form $e\ddot{\mathbf{v}}\mathbf{v}/rc^3$ which can be called 'quadrupole radiation'. In still higher order, terms such as $e\ddot{\mathbf{v}}\mathbf{v}^2/rc^4$ appear. In this manner the approximation can be carried to arbitrarily high order. (The following symbols, have been employed: \mathfrak{E} , \mathfrak{H} are field strengths at a given point, \mathbf{r} the vector between this point and the position of the electron, \mathbf{v} the velocity and e the charge of the electron).

One may inquire about the form these higher order terms would assume in quantum theory. The higher order approximations can easily be calculated in classical theory if the motion of the electron is

¹ H. A. Kramers, Nature **113** (1924) 673.

² M. Born, Zs. f. Phys. **26** (1924) 379. H. A. Kramers and W. Heisenberg, Zs. f. Phys. **31** (1925) 681. M. Born and P. Jordan, Zs. f. Phys. (in course of publication) [33 (1925) 479; paper 7a].

given in Fourier expansion, and one would expect a similar result in quantum theory. This point has nothing to do with electrodynamics but rather – and this seems to be particularly important – is of a purely kinematic nature. We may pose the question in its simplest form thus: If instead of a classical quantity $x(t)$ we have a quantum-theoretical quantity, what quantum-theoretical quantity will appear in place of $x(t)^2$?

Before we can answer this question, it is necessary to bear in mind that in quantum theory it has not been possible to associate the electron with a point in space, considered as a function of time, by means of observable quantities. However, even in quantum theory it is possible to ascribe to an electron the emission of radiation. In order to characterize this radiation we first need the frequencies which appear as functions of two variables. In quantum theory these functions are of the form

$$\nu(n, n - \alpha) = \frac{1}{h} \{W(n) - W(n - \alpha)\},$$

and in classical theory of the form

$$\nu(n, \alpha) = \alpha \nu(n) = \alpha \frac{1}{h} \frac{dW}{dn}.$$

(Here one has $nh=J$, where J is one of the canonical constants).

As characteristic for the comparison between classical and quantum theory with respect to frequency, one can write down the combination relations:

Classical:

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

Quantum-theoretical:

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

or

$$\nu(n - \beta, n - \alpha - \beta) + \nu(n, n - \beta) = \nu(n, n - \alpha - \beta).$$

In order to complete the description of radiation it is necessary to have not only the frequencies but also the amplitudes. The amplitudes may be treated as complex vectors, each determined by six independent components, and they determine both the polarization and the phase. As the amplitudes are also functions of the two variables

n and α , the corresponding part of the radiation is given by the following expressions:

Quantum-theoretical:

$$\text{Re}\{\mathfrak{A}(n, n - \alpha) e^{i\omega(n, n-\alpha)t}\}. \quad (1)$$

Classical:

$$\text{Re}\{\mathfrak{A}_\alpha(n) e^{i\omega(n)\alpha t}\}. \quad (2)$$

At first sight the phase contained in \mathfrak{A} would seem to be devoid of physical significance in quantum theory, since in this theory frequencies are in general not commensurable with their harmonics. However, we shall see presently that also in quantum theory the phase has a definite significance which is analogous to its significance in classical theory. If we now consider a given quantity $x(t)$ in classical theory, this can be regarded as represented by a set of quantities of the form

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

which, depending upon whether the motion is periodic or not, can be combined into a sum or integral which represents $x(t)$:

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

or

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

A similar combination of the corresponding quantum-theoretical quantities seems to be impossible in a unique manner and therefore not meaningful, in view of the equal weight of the variables n and $n - \alpha$. However, one may readily regard the ensemble of quantities $\mathfrak{A}(n, n - \alpha) e^{i\omega(n, n-\alpha)t}$ as a representation of the quantity $x(t)$ and then attempt to answer the above question: how is the quantity $x(t)^2$ to be represented?

The answer in classical theory is obviously:

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

or

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

so that

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

or, respectively,

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

In quantum theory, it seems that the simplest and most natural assumption would be to replace equations (3) and (4) by:

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

or

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

and in fact this type of combination is an almost necessary consequence of the frequency combination rules. On making assumptions (7) and (8), one recognizes that the phases of the quantum-theoretical \mathfrak{A} have just as great a physical significance as their classical analogues. Only the origin of the time scale and hence a phase factor common to all the \mathfrak{A} is arbitrary and accordingly devoid of physical significance, but the phases of the individual \mathfrak{A} enter in an essential manner into the quantity \mathfrak{B} .¹ A geometrical interpretation of such quantum-theoretical phase relations in analogy with those of classical theory seems at present scarcely possible.

If we further ask for a representation for the quantity $x(t)^3$ we find without difficulty:

Classical:

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

Quantum-theoretical:

$$\mathfrak{C}(n, n - \gamma) =$$

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

or the corresponding integral forms.

¹ Cf. also H. A. Kramers and W. Heisenberg, loc.cit. The phases enter essentially into the expressions used there for the induced scattering moment.

In a similar manner, one can find a quantum-theoretical representation for all quantities of the form $x(t)^n$, and if any function $f[x(t)]$ is given, one can always find the corresponding quantum-theoretical expression, provided the function can be expanded as a power series in x . A significant difficulty arises, however, if we consider two quantities $x(t)$, $y(t)$, and ask after their product $x(t)y(t)$. If $x(t)$ is characterized by \mathfrak{A} , and $y(t)$ by \mathfrak{B} , we obtain the following representations for $x(t)y(t)$:

Classical:

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

Quantum-theoretical:

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

Whereas in classical theory $x(t)y(t)$ is always equal to $y(t)x(t)$, this is not necessarily the case in quantum theory. In special instances, e.g., in the expression $x(t)x(t)^2$, this difficulty does not arise.

If, as in the question posed at the beginning of this section, one is interested in products of the form $v(t)\dot{v}(t)$, then in quantum theory this product $v\dot{v}$ should be replaced by $\frac{1}{2}(v\dot{v} + \dot{v}v)$, in order that $v\dot{v}$ be the differential coefficient of $\frac{1}{2}v^2$. In a similar manner it would always seem possible to find natural expressions for the quantum-theoretical mean values, though they may be even more hypothetical than the formulae (7) and (8).

Apart from the difficulty just mentioned, formulae of the type (7), (8) should quite generally also suffice to express the interaction of the electrons in an atom in terms of the characteristic amplitudes of the electrons.

2. After these considerations which were concerned with the kinematics of quantum theory, we turn our attention to the dynamical problem which aims at the determination of the \mathfrak{A} , \mathfrak{v} , W from the given forces of the system. In earlier theory this problem was solved in two stages:

1. Integration of the equation of motion

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

2. Determination of the constants for periodic motion through

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

If one seeks to construct a quantum-mechanical formalism corresponding as closely as possible to that of classical mechanics, it is very natural to take over the equation of motion (11) directly into quantum theory. At this point, however, it is necessary – in order not to depart from the firm foundation provided by those quantities that are in principle observable – to replace the quantities \ddot{x} and $f(x)$ by their quantum-theoretical representatives, as given in § 1. In classical theory it is possible to obtain the solution of (11) by first expressing x as a Fourier series or Fourier integral with undetermined coefficients (and frequencies). In general, we then obtain an infinite set of equations containing infinitely many unknowns, or integral equations, which can be reduced to simple recursive relations for the α in special cases only. In quantum theory we are at present forced to adopt this method of solving equation (11) since, as has been said before, it was not possible to define a quantum-theoretical function directly analogous to the function $x(n, t)$.

Consequently the quantum-theoretical solution of (11) is only possible in the simplest cases. Before we consider such simple examples, let us give a quantum-theoretical re-interpretation of the determination, from (12), of the constant of periodic motion. We assume that (classically) the motion is periodic:

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

hence

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

and

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

Furthermore, since $a_{-\alpha}(n) = \overline{a_\alpha(n)}$, as x is to be real, it follows that

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

In the earlier theory this phase integral was usually set equal to an integer multiple of h , i.e., equal to nh , but such a condition does

not fit naturally into the dynamical calculation. It appears, even when regarded from the point of view adopted hitherto, arbitrary in the sense of the correspondence principle, because from this point of view the J are determined only up to an additive constant as multiples of \hbar . Instead of (14) it would be more natural to write

$$\frac{d}{dn} (nh) = \frac{d}{dn} \oint mx^2 dt,$$

that is,

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

Such a condition obviously determines the α_α only to within a constant, and in practice this indeterminacy has given rise to difficulties due to the occurrence of half-integral quantum numbers.

If we look for a quantum-theoretical relation corresponding to (14) and (15) and containing observable quantities only, the uniqueness which had been lost is automatically restored.

We have to admit that only equation (15) has a simple quantum-theoretical reformulation which is related to *Kramers'* dispersion theory:¹

$$\hbar = 4\pi m \sum_0^{\infty} \alpha \{ |a(n, n + \alpha)|^2 \omega(n, n + \alpha) - |a(n, n - \alpha)|^2 \omega(n, n - \alpha) \}. \quad (16)$$

Yet this relation suffices to determine the a uniquely since the undetermined constant contained in the quantities a is automatically fixed by the condition that a ground state should exist, from which no radiation is emitted. Let this ground state be denoted by n_0 ; then we should have $a(n_0, n_0 - \alpha) = 0$ (for $\alpha > 0$). Hence we may expect that the question of half-integer or integer quantization does not arise in a theoretical quantum mechanics based only upon relations between observable quantities.

Equations (11) and (16), if soluble, contain a complete determination not only of frequencies and energy values, but also of quantum-theoretical transition probabilities. However, at present the actual mathematical solution can be obtained only in the simplest cases. In many systems, e.g. the hydrogen atom, a particular complication

¹ This relation has already been derived from dispersion considerations by W. Kuhn, Zs. Phys. **33** (1925) 408, and W. Thomas, Naturwiss. **13** (1925) 627.

arises because the solutions correspond to motion which is partly periodic and partly aperiodic. As a consequence of this property, the quantum-theoretical series (7), (8) and equation (16) decompose into a sum and an integral. Quantum-mechanically such a decomposition into 'periodic and aperiodic motion' cannot be carried out in general.

Nevertheless, one could regard equations (11) and (16) as a satisfactory solution, at least in principle, of the dynamical problem if it were possible to show that this solution agrees with (or at any rate does not contradict) the quantum-mechanical relationships which we know at present. It should, for instance, be established that the introduction of a small perturbation into a dynamical problem leads to additional terms in the energy, or frequency, of the type found by *Kramers* and *Born* – but not of the type given by classical theory. Furthermore, one should also investigate whether equation (11) in the present quantum-theoretical form would in general give rise to an energy integral $\frac{1}{2}m\dot{x}^2 + U(x) = \text{const.}$, and whether the energy so derived satisfies the condition $\Delta W = h\nu$, in analogy with the classical condition $\nu = \partial W / \partial J$. A general answer to these questions would elucidate the intrinsic connections between previous quantum-mechanical investigations and pave the way toward a consistent quantum-mechanics based solely upon observable quantities. Apart from a general connection between Kramer's dispersion formula and equations (11) and (16), we can answer the above questions only in very special cases which may be solved by simple recursion relations.

The general connection between *Kramers'* dispersion theory and our equations (11) and (16) is as follows. From equation (11) (more precisely, from the quantum-theoretical analogue) one finds, just as in classical theory, that the oscillating electron behaves like a free electron when acted upon by light of much higher frequency than any eigenfrequency of the system. This result also follows from Kramers' dispersion theory if in addition one takes account of equation (16). In fact, *Kramers* finds for the moment induced by a wave of the form $E \cos 2\pi\nu t$:

$$M = e^2 E \cos 2\pi\nu t \frac{2}{h} \sum_0^\infty \alpha \left\{ \frac{|a(n, n + \alpha)|^2 \nu(n, n + \alpha)}{\nu^2(n, n + \alpha) - \nu^2} - \frac{|a(n, n - \alpha)|^2 \nu(n, n - \alpha)}{\nu^2(n, n - \alpha) - \nu^2} \right\},$$

so that for $\nu \gg v(n, n+\alpha)$,

$$M = -\frac{2Ee^2 \cos 2\pi\nu t}{v^2 h} \sum_0^\infty \sum_\alpha \{ |a(n, n+\alpha)|^2 \nu(n, n+\alpha) \\ - |a(n, n-\alpha)|^2 \nu(n, n-\alpha) \},$$

which, due to equation (16), becomes

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

3. As a simple example, the anharmonic oscillator will now be treated:

$$\ddot{x} + \omega_0^2 x + \lambda x^2 = 0. \quad (17)$$

Classically, this equation is satisfied by a solution of the form

$x = \lambda a_0 + a_1 \cos \omega t + \lambda a_2 \cos 2\omega t + \lambda^2 a_3 \cos 3\omega t + \dots \lambda^{\tau-1} a_\tau \cos \tau \omega t$, where the a are power series in λ , the first terms of which are independent of λ . Quantum-theoretically we attempt to find an analogous expression, representing x by terms of the form

$$\begin{aligned} & \lambda a(n, n); \quad a(n, n-1) \cos \omega(n, n-1)t; \\ & \lambda a(n, n-2) \cos \omega(n, n-2)t; \\ & \dots \lambda^{\tau-1} a(n, n-\tau) \cos \omega(n, n-\tau)t \dots \end{aligned}$$

The recursion formulae which determine the a and ω (up to, but excluding, terms of order λ) according to equations (3), (4) or (7), (8) are:

Classical:

$$\begin{aligned} \omega_0^2 a_0(n) + \frac{1}{2} a_1^2(n) &= 0; \\ -\omega^2 + \omega_0^2 &= 0; \\ (-4\omega^2 + \omega_0^2) a_2(n) + \frac{1}{2} a_1^2 &= 0; \\ (-9\omega^2 + \omega_0^2) a_3(n) + a_1 a_2 &= 0; \\ \dots &\dots \end{aligned} \quad (18)$$

Quantum-theoretical:

$$\begin{aligned} \omega_0^2 a_0(n) + \frac{1}{4} [a^2(n+1, n) + a^2(n, n-1)] &= 0; \\ -\omega^2(n, n-1) + \omega_0^2 &= 0; \\ [-\omega^2(n, n-2) + \omega_0^2] a(n, n-2) + \frac{1}{2} [a(n, n-1) a(n-1, n-2)] &= 0; \\ [-\omega^2(n, n-3) + \omega_0^2] a(n, n-3) + \frac{1}{2} [a(n, n-1) a(n-1, n-3) + a(n, n-2) a(n-2, n-3)] &= 0; \\ \dots &\dots \end{aligned} \quad (19)$$

The additional quantum condition is:

Classical ($J = nh$):

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

Quantum-theoretical:

$$h = \pi m \sum_0^{\infty} [|a(n + \tau, n)|^2 \omega(n + \tau, n) - |a(n, n - \tau)|^2 \omega(n, n - \tau)].$$

We obtain in first order, both classically and quantum-mechanically

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

In quantum theory, the constant in equation (20) can be determined from the condition that $a(n_0, n_0 - 1)$ should vanish in the ground state. If we number the n in such a way that in the ground state n is zero, i.e. $n_0 = 0$, then $a^2(n, n - 1) = nh/\pi m \omega_0$.

It thus follows from the recursive relations (18) that in classical theory the coefficient a_τ has (to first order in λ) the form $\kappa(\tau)n^{\frac{1}{2}\tau}$ where $\kappa(\tau)$ represents a factor independent of n . In quantum theory, equation (19) implies

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

where $\kappa(\tau)$ is the same proportionality factor, independent of n . Naturally, for large values of n the quantum-theoretical value of a_τ tends asymptotically to the classical value.

An obvious next step would be to try inserting the classical expression for the energy $\frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega_0^2x^2 + \frac{1}{3}m\lambda x^3 = W$, because in the present first-approximation calculation it actually is constant, even when treated quantum-theoretically. Its value is given by (19), (20) and (21) as:

Classical:

$$W = nh\omega_0/2\pi. \quad (22)$$

Quantum-theoretical, from (7) and (8):

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

(terms of order λ^2 have been excluded).

Thus from the present viewpoint, even the energy of a harmonic oscillator is not given by 'classical mechanics', i.e., by equation (22), but has the form (23).

The more precise calculation, taking into account higher order approximations in W , a , ω will now be carried out for the simpler example of an anharmonic oscillator $\ddot{x} + \omega_0^2 x + \lambda x^3 = 0$.

Classically, one can in this case set

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

quantum-theoretically we attempt to set by analogy

$$a(n, n - 1) \cos \omega(n, n - 1)t; \quad \lambda a(n, n - 3) \cos \omega(n, n - 3)t; \quad \dots$$

The quantities a are once more power series in λ whose first term has the form, as in equation (21),

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

as one finds by evaluating the equations corresponding to (18) and (19).

If the evaluation of ω and a from equations (18) and (19) is carried out to order λ^2 or λ respectively, one obtains

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

$$a(n, n - 1) = \sqrt{\frac{nh}{\pi\omega_0 m}} \left(1 - \lambda \frac{3nh}{16\pi\omega_0^3 m} + \dots \right). \quad (25)$$

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

The energy, defined as the constant term in the expression

$$\frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega_0^2 x^2 + \frac{1}{4}m\lambda x^4,$$

(I could not prove in general that all periodic terms actually vanish,

but this was the case for all terms evaluated) turns out to be

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

This energy can also be determined using the *Kramers-Born* approach by treating the term $\frac{1}{4}m\lambda x^4$ as a perturbation to the harmonic oscillator. The fact that one obtains exactly the same result (27) seems to me to furnish remarkable support for the quantum-mechanical equations which have here been taken as basis. Furthermore, the energy calculated from (27) satisfies the relation (cf. eq. 24):

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

which can be regarded as a necessary condition for the possibility of a determination of the transition probabilities according to equations (11) and (16).

In conclusion we consider the case of a rotator and call attention to the relationship of equations (7), (8) to the intensity formulae for the Zeeman effect¹ and for multiplets.²

Consider the rotator as represented by an electron which circles a nucleus with constant distance a . Both classically and quantum-theoretically, the 'equations of motion' simply state that the electron describes a plane, uniform rotation at a distance a and with angular velocity ω about the nucleus. The 'quantum condition' (16) yields, according to (12),

$$\hbar = \frac{d}{dn} (2\pi ma^2\omega),$$

and according to (16)

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

¹ S. Goudsmit and R. de L. Kronig, Naturwiss. **13** (1925) 90; H. Hönl, Zs. f. Phys. **31** (1925) 340.

² R. de L. Kronig, Zs. f. Phys. **31** (1925) 885; A. Sommerfeld and H. Hönl, Sitzungsber. d. Preuss. Akad. d. Wiss. (1925) 141; H. N. Russell, Nature **115** (1925) 835.

from which, in both cases, it follows that

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

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

$$\omega(n, n - 1) = \frac{hn}{2\pi ma^2}. \quad (28)$$

The energy is

$$W = \frac{1}{2}mv^2,$$

or, from equations (7), (8),

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

which again satisfies the condition $\omega(n, n-1) = (2\pi/h)[W(n) - W(n-1)]$.

As support for the validity of the formulae (28) and (29), which differ from those of the usual theory, one might mention that, according to Kratzer,¹ many band spectra (including spectra for which the existence of an electron momentum is improbable) seem to require formulae of type (28), (29), which, in order to avoid rupture with the classical theory of mechanics, one had hitherto endeavoured to explain through half-integer quantization.

In order to arrive at the *Goudsmit-Kronig-Hönl* formula for the rotator we have to leave the field of problems having one degree of freedom. We assume that the rotator has a direction in space which is subject to a very slow precession ω about the z -axis of an external field. Let the quantum number corresponding to this precession be m . The motion is then represented by the quantities

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

The equations of motion are simply

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

¹ Cf. for example, B. A. Kratzer, Sitzungsber. d. Bayr. Akad. (1922) p. 107

Because of (7) this leads to¹

$$\begin{aligned} \frac{1}{2}\{ & \frac{1}{2}a^2(n, n-1; m, m) + b^2(n, n-1; m, m-1) + b^2(n, n-1; m, m+1) \\ & + \frac{1}{2}a^2(n+1, n; m, m) + b^2(n+1, n; m-1, m) \\ & + b^2(n+1, n; m+1, m) \} = a^2. \end{aligned} \quad (30)$$

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

One also has the quantum condition from (16):

$$\begin{aligned} & 2\pi m\{b^2(n, n-1; m, m-1)\omega(n, n-1) \\ & - b^2(n, n-1; m-1, m)\omega(n, n-1)\} = (m + \text{const})\hbar. \end{aligned} \quad (32)$$

The classical relations corresponding to these equations are

$$\begin{aligned} & \frac{1}{2}a_0^2 + b_1^2 + b_{-1}^2 = a^2; \\ & \frac{1}{4}a_0^2 = b_1 b_{-1}; \\ & 2\pi m(b_{+1}^2 - b_{-1}^2)\omega = (m + \text{const})\hbar. \end{aligned} \quad (33)$$

They suffice (up to the unknown constant added to m) to determine a_0, b_1, b_{-1} uniquely.

The simplest solution of the quantum-theoretical equations (30), (31), (32) which presents itself is:

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

These expressions agree with the formulae of *Goudsmid, Kronig and Hönl*. It is, however, not easily seen that these expressions represent the *only* solution of equations (30), (31), (32), though this would seem likely to me from consideration of the boundary conditions (vanishing

¹ Equation (30) is essentially identical with the *Ornstein-Burger* sum rules.

of a and b at the 'boundary'; cf. the papers of *Kronig, Sommerfeld* and *Hönl, Russell* quoted above).

Considerations similar to the above, applied to the multiplet intensity formulae, lead to the result that these intensity rules are in agreement with equations (7) and (16). This finding may again be regarded as furnishing support for the validity of the kinematic equation (7).

Whether a method to determine quantum-theoretical data using relations between observable quantities, such as that proposed here, can be regarded as satisfactory in principle, or whether this method after all represents far too rough an approach to the physical problem of constructing a theoretical quantum mechanics, an obviously very involved problem at the moment, can be decided only by a more intensive mathematical investigation of the method which has been very superficially employed here.