

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*<sup>1</sup> together with its extensions in recent papers<sup>2</sup> 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

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

but additional terms occur in the next order of approximation, e.g. terms of the form  $e\dot{\mathfrak{v}}\mathfrak{v}/rc^3$  which can be called 'quadrupole radiation'. In still higher order, terms such as  $e\dot{\mathfrak{v}}\mathfrak{v}^2/rc^4$  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,  $\mathfrak{r}$  the vector between this point and the position of the electron,  $\mathfrak{v}$  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

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

<sup>2</sup> 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  $x(t)$ ?<sup>2</sup>

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  $\alpha$ , the corresponding part of the radiation is given by the following expressions:

Quantum-theoretical:

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

Classical:

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

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  $x(t)$ :

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

or

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

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

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

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:

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

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  $\mathfrak{B}$ .<sup>1</sup> 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  $x(t)$ <sup>3</sup> 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:

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

or the corresponding integral forms.

<sup>1</sup> 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:

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

Quantum-theoretical:

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

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  $\mathfrak{A}$ ,  $\nu$ ,  $W$  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  $\mathfrak{A}$  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  $h$ . Instead of (14) it would be more natural to write

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

that is,

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

Such a condition obviously determines the  $a_\alpha$  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:<sup>1</sup>

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

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

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