

QUANTUM-THEORETICAL RE-INTERPRETATION
OF KINEMATIC AND MECHANICAL RELATIONS

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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

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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

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

but additional terms occur in the next order of approximation, e.g. terms of the form $e\dot{\mathbf{v}}\dot{\mathbf{v}}/rc^3$ which can be called 'quadrupole radiation'. In still higher order, terms such as $e\dot{\mathbf{v}}\dot{\mathbf{v}}^2/rc^4$ 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, $\dot{\mathbf{v}}$ 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 $n\hbar = J$, 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:

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

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 $\mathfrak{B}$.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:

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

or the corresponding integral forms.

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:

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

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 $\mathfrak{A}$, ν , 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_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

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

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 $\nu \gg \nu(n, n + \alpha)$,

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

which, due to equation (16), becomes

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

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:

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

Quantum-theoretical:

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

The additional quantum condition is:

Classical ($J=n\hbar$):

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

Quantum-theoretical:

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

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

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

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 $a^2(n, n-1)=n\hbar/\pi m \omega_0$.

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 $\frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega_0^2 x^2 + \frac{1}{3}m\lambda x^3 = W$, 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:

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

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

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

(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

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

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

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

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

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

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):

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

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),

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

and according to (16)

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

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

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

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

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

The energy is

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

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

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

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 ϑ 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

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

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):

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

The classical relations corresponding to these equations are

$$\begin{aligned} \frac{1}{2}a_0^2 + b_1^2 + b_{-1}^2 &= a^2; \\ \frac{1}{4}a_0^2 &= b_1b_{-1}; \\ 2\pi m(b_{+1}^2 - b_{-1}^2)\omega &= (m + \text{const})h. \end{aligned} \quad (33)$$

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 *Goudsmit*, *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.

Understanding Heisenberg's "magical" paper of July 1925: A new look at the calculational details

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Understanding Heisenberg's "magical" paper of July 1925: A new look at the calculational details

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In July 1925 Heisenberg published a paper that ushered in the new era of quantum mechanics. This epoch-making paper is generally regarded as being difficult to follow, partly because Heisenberg provided few clues as to how he arrived at his results. We give details of the calculations of the type that Heisenberg might have performed. As an example we consider one of the anharmonic oscillator problems considered by Heisenberg, and use our reconstruction of his approach to solve it up to second order in perturbation theory. The results are precisely those obtained in standard quantum mechanics, and we suggest that a discussion of the approach, which is based on the direct calculation of transition frequencies and amplitudes, could usefully be included in undergraduate courses on quantum mechanics. © 2004 American Association of Physics Teachers.

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I. INTRODUCTION

Heisenberg's paper of July 1925¹ on "Quantum-mechanical reinterpretation of kinematic and mechanical relations,"^{2,3} was the breakthrough that quickly led to the first complete formulation of quantum mechanics.^{4–6} Despite its undoubtedly crucial historical role, Heisenberg's approach in this paper is not generally followed in undergraduate quantum mechanics courses, in contrast, for example, to Einstein's approach in the teaching of relativity. Indeed Heisenberg's paper is widely regarded as being difficult to understand and of mainly historical interest today. For example, Weinberg⁷ has written that "If the reader is mystified at what Heisenberg was doing, he or she is not alone. I have tried several times to read the paper that Heisenberg wrote on returning from Heligoland, and, although I think I understand quantum mechanics, I have never understood Heisenberg's motivations for the mathematical steps in his paper. Theoretical physicists in their most successful work tend to play one of two roles: they are either *sages* or *magicians* ... It is usually not difficult to understand the papers of sage-physicists, but the papers of magician-physicists are often incomprehensible. In this sense, Heisenberg's 1925 paper was pure magic."

There have been many discussions aimed at elucidating the main ideas in Heisenberg's paper of which Refs. 3 and 8–18 represent only a partial selection.¹⁹ Of course, it may not be possible to render completely comprehensible the mysterious processes whereby physicists "jump over all intermediate steps to a new insight about nature."²⁰ In our opinion, however, one of the main barriers to understanding Heisenberg's paper is a more prosaic one: namely, he gave remarkably few details of the calculations he performed.

In Sec. II we briefly review Heisenberg's reasoning in setting up his new calculational method. Then we present in Sec. III the details of a calculation typical of those we conjecture that he performed. Our reconstruction is based on the

assumption that, having formulated a method that was capable of determining the relevant physical quantities (the transition frequencies and amplitudes), Heisenberg then applied it to various simple mechanical systems, without any further recourse to the kind of "inspired guesswork" that characterized the old quantum theory. Surprisingly, this point of view appears to be novel. For example, MacKinnon¹⁰ and Mehra and Rechenberg¹¹ have suggested that Heisenberg arrived at the crucial recursion relations [see Eqs. (33)–(36) in Sec. III B] by essentially guessing the appropriate generalization of their classical counterparts. We are unaware of any evidence that can settle the issue. In any case, our analysis shows that it is possible to read Heisenberg's paper as providing a complete (if limited) calculational method, the results of which are consistent with those of standard quantum mechanics. We also stress both the correctness and the practicality of what we conjecture to be Heisenberg's calculational method. We hope that our reappraisal will stimulate instructors to include at least some discussion of it in their undergraduate courses.

II. HEISENBERG'S TRANSITION AMPLITUDE APPROACH

A. Quantum kinematics

Heisenberg began his paper with a programmatic call^{21,22} to "discard all hope of observing hitherto unobservable quantities, such as the position and period of the electron," and instead to "try to establish a theoretical quantum mechanics, analogous to classical mechanics, but in which only relations between observable quantities occur." As an example of such latter quantities, he immediately pointed to the energies $W(n)$ of the Bohr stationary states, together with the associated Einstein–Bohr frequencies²³

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

and noted that these frequencies, which characterize the radiation emitted in the transition $n \rightarrow n - \alpha$, depend on two variables. An example of a quantity he wished to exclude from the new theory is the time-dependent position coordinate $x(t)$. In considering what might replace it, he turned to the probabilities for transitions between stationary states.

Consider a simple one-dimensional model of an atom consisting of an electron undergoing periodic motion, which is the type of system studied by Heisenberg. For a state characterized by the label n , the fundamental frequency $\omega(n)$, and the coordinate $x(n, t)$, we can represent $x(n, t)$ as a Fourier series

$$x(n, t) = \sum_{\alpha=-\infty}^{\infty} X_{\alpha}(n) e^{i\alpha\omega(n)t}, \quad (2)$$

where α is an integer.²⁴ According to classical theory, the energy emitted per unit time (the power) in a transition corresponding to the α th harmonic $\alpha\omega(n)$ is²⁵

$$-\left(\frac{dE}{dt}\right)_{\alpha} = \frac{e^2}{3\pi\epsilon_0 c^3} [\alpha\omega(n)]^4 |X_{\alpha}(n)|^2. \quad (3)$$

In the quantum theory, however, the transition frequency corresponding to the classical $\alpha\omega(n)$ is, in general, not a simple multiple of a fundamental frequency, but is given by Eq. (1), so that $\alpha\omega(n)$ is replaced by $\omega(n, n - \alpha)$. Correspondingly, Heisenberg introduced the quantum analogue of $X_{\alpha}(n)$, written (in our notation) as $X(n, n - \alpha)$.²⁷ Furthermore, the left-hand side of Eq. (3) has to be replaced by the product of the transition probability per unit time, $P(n, n - \alpha)$, and the emitted energy $\hbar\omega(n, n - \alpha)$. Thus Eq. (3) becomes

$$P(n, n - \alpha) = \frac{e^2}{3\pi\epsilon_0 \hbar c^3} [\omega(n, n - \alpha)]^3 |X(n, n - \alpha)|^2. \quad (4)$$

It is the transition amplitudes $X(n, n - \alpha)$ which Heisenberg took to be “observable;” like the transition frequencies, they depend on two discrete variables.²⁸

Equation (4) refers, however, to only one specific transition. For a full description of atomic dynamics (as then conceived), we need to consider all the quantities $X(n, n - \alpha) \exp[i\omega(n, n - \alpha)t]$. In the classical case, the terms $X_{\alpha}(n) \exp[i\alpha\omega(n)t]$ may be combined to yield $x(t)$ via Eq. (2). But in the quantum theory, Heisenberg wrote²⁹ that 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 $n - \alpha$ [that is, in the amplitude $X(n, n - \alpha)$ and frequency $\omega(n, n - \alpha)$] ... However, one may readily regard the ensemble of quantities $X(n, n - \alpha) \exp[i\omega(n, n - \alpha)t]$ as a representation of the quantity $x(t)$...” This way of representing $x(t)$, that is, as we would now say, by a matrix, is the first of Heisenberg’s “magical jumps,” and surely a very large one. Representing $x(t)$ in this way seems to be the sense in which Heisenberg considered that he was offering a “reinterpretation of kinematic relations.”

Heisenberg immediately posed the question: how is the quantity $x(t)$ ² to be represented? In classical theory, the answer is straightforward. From Eq. (2) we obtain

$$[x(t)]^2 = \sum_{\alpha} \sum_{\alpha'} X_{\alpha}(n) X_{\alpha'}(n) e^{i(\alpha + \alpha')\omega(n)t}. \quad (5)$$

We set $\beta = \alpha + \alpha'$, and rewrite Eq. (5) as

$$[x(t)]^2 = \sum_{\beta} Y_{\beta}(n) e^{i\beta\omega(n)t}, \quad (6)$$

where

$$Y_{\beta}(n) = \sum_{\alpha} X_{\alpha}(n) X_{\beta-\alpha}(n). \quad (7)$$

Thus $[x(t)]^2$ is represented classically (via a Fourier series) by the set of quantities $Y_{\beta}(n) \exp[i\beta\omega(n)t]$, the frequency $\beta\omega(n)$ being the simple combination $[\alpha\omega(n) + (\beta - \alpha)\omega(n)]$. In quantum theory, the corresponding representative quantities must be written as $Y(n, n - \beta) \exp[i\omega(n, n - \beta)t]$, and the question is what is the analogue of Eq. (7)?

The crucial difference in the quantum case is that the frequencies do not combine in the same way as the classical harmonics, but rather in accordance with the Ritz combination principle:

$$\omega(n, n - \alpha) + \omega(n - \alpha, n - \beta) = \omega(n, n - \beta), \quad (8)$$

which is consistent with Eq. (1). Thus in order to end up with the particular frequency $\omega(n, n - \beta)$, it seems “almost necessary” (in Heisenberg’s words³⁰) to combine the quantum amplitudes in such a way as to ensure the frequency combination Eq. (8), that is, as

$$Y(n, n - \beta) e^{i\omega(n, n - \beta)t} = \sum_{\alpha} X(n, n - \alpha) e^{i\omega(n, n - \alpha)t} \times X(n - \alpha, n - \beta) e^{i\omega(n - \alpha, n - \beta)t}, \quad (9)$$

or

$$Y(n, n - \beta) = \sum_{\alpha} X(n, n - \alpha) X(n - \alpha, n - \beta), \quad (10)$$

which is Heisenberg’s rule for multiplying transition amplitudes. Note particularly that the replacements $X_{\alpha}(n) \rightarrow X(n, n - \alpha)$, and similarly for $Y_{\beta}(n)$ and $X_{\beta-\alpha}(n)$ in Eq. (7), produce a quite different result.

Heisenberg indicated the simple extension of the rule given in Eq. (10) to higher powers $[x(t)]^n$, but noticed at once³¹ that a “significant difficulty arises, however, if we consider two quantities $x(t), y(t)$ and ask after their product $x(t)y(t)$... 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.” Heisenberg used the word “difficulty” three times in referring to this unexpected consequence of his multiplication rule, but it very quickly became clear that the non-commutativity (in general) of kinematical quantities in quantum theory was the essential new idea in the paper.

Born recognized Eq. (10) as matrix multiplication (something unknown to Heisenberg in July 1925), and he and Jordan rapidly produced the first paper⁴ to state the fundamental commutation relation (in modern notation)

$$\hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar. \quad (11)$$

Dirac’s paper followed soon after,⁵ and then the paper of Born, Heisenberg, and Jordan.⁶

The economy and force of Heisenberg's argument in reaching Eq. (10) is remarkable, and it is at least worth considering whether presenting it to undergraduates might help them to understand the “almost necessity” of non-commuting quantities in quantum theory.

B. Quantum dynamics

Having identified the transition amplitudes $X(n, n-\alpha)$ and frequencies $\omega(n, n-\alpha)$ as the observables of interest in the new theory, Heisenberg then turned his attention to how they could be determined from the dynamics of the system. In the old quantum theory, this determination would have been done in two stages: by integration of the equation of motion

$$\ddot{x} + f(x) = 0, \quad (12)$$

and by determining the constants of the periodic motion through the “quantum condition”

$$\oint p dq = \oint m \dot{x}^2 dt = J (= nh), \quad (13)$$

where the integral is evaluated over one period. In regard to Eq. (12), Heisenberg wrote³² that it is “very natural” to take the classical equation of motion over to quantum theory by replacing the classical quantities $x(t)$ and $f(x)$ by their kinematical reinterpretations,³³ as in Sec. II A (or, as we would say today, by taking matrix elements of the corresponding operator equation of motion). He noted that in the classical case a solution can be obtained by expressing $x(t)$ as a Fourier series, substitution of which into the equation of motion leads (in special cases) to a set of recursion relations for the Fourier coefficients. In the quantum theory, Heisenberg wrote that³² “we are at present forced to adopt this method of solving equation Eq. (12) [his Eq. (H11)] ... since it was not possible to define a quantum-theoretical function analogous to the [classical] function $x(n, t)$.” In Sec. III we shall consider the simple example (the first of those chosen by Heisenberg) $f(x) = \omega_0^2 x + \lambda x^2$, and obtain the appropriate recursion relations in the classical and the quantum cases.

A quantum-theoretical reinterpretation of Eq. (13) is similarly required in terms of the transition amplitudes $X(n, n-\alpha)$. In the classical case, the substitution of Eq. (2) into Eq. (13) gives

$$\oint m \dot{x}^2 dt = 2\pi m \sum_{\alpha=-\infty}^{\infty} |X_{\alpha}(n)|^2 \alpha^2 \omega(n) = nh, \quad (14)$$

using $X_{\alpha}(n) = [X_{-\alpha}(n)]^*$. Heisenberg argued that Eq. (14) appeared arbitrary in the sense of the correspondence principle, because the latter determined J only up to an additive constant (times h). He therefore replaced Eq. (14) by the derivative form [Eq. (H15)]

$$h = 2\pi m \sum_{\alpha=-\infty}^{\infty} \alpha \frac{d}{dn} (\alpha |X_{\alpha}(n)|^2 \omega(n)). \quad (15)$$

The summation can alternatively be written as over positive values of α , replacing $2\pi m$ by $4\pi m$. In another crucial jump, Heisenberg then replaced the differential in Eq. (15) by a difference, giving

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

which is Eq. (H16) in our notation.³⁴ As he later recalled, he had noticed that “if I wrote down this [presumably Eq. (15)] and tried to translate it according to the scheme of dispersion theory, I got the Thomas-Kuhn sum rule [Eq. (16)]^{35,36}. And that is the point. Then I thought, That is apparently how it is done.”³⁷

By “the scheme of dispersion theory,” Heisenberg referred to what Jammer³⁸ calls Born's correspondence rule, namely³⁹

$$\alpha \frac{\partial \Phi(n)}{\partial n} \leftrightarrow \Phi(n) - \Phi(n-\alpha), \quad (17)$$

or rather to its iteration to the form⁴⁰

$$\alpha \frac{\partial \Phi(n, \alpha)}{\partial n} \leftrightarrow \Phi(n+\alpha, n) - \Phi(n, n-\alpha), \quad (18)$$

as used in the Kramers–Heisenberg theory of dispersion.^{41,42} It took Born only a few days to show that Heisenberg's quantum condition, Eq. (16), was the diagonal matrix element of Eq. (11), and to guess⁴³ that the off-diagonal elements of $\hat{x}\hat{p} - \hat{p}\hat{x}$ were zero, a result that was shown to be compatible with the equations of motion by Born and Jordan.⁴

At this point it is appropriate to emphasize that Heisenberg's transition amplitude $X(n, n-\alpha)$ is the same as the quantum-mechanical matrix element $\langle n-\alpha | \hat{x} | n \rangle$, where $|n\rangle$ is the eigenstate with energy $W(n)$. The relation of Eq. (16) to the fundamental commutator Eq. (11) is discussed briefly in Appendix A.

Heisenberg noted⁴⁴ that the undetermined constant still contained in the quantities X of Eq. (16) [assuming the frequencies known from Eq. (12)] would be determined by the condition that a ground state should exist, from which no radiation is emitted [see Eqs. (51) and (52) below]. He therefore summarized the state of affairs thus far by the statement⁴⁴ that Eqs. (12) and (16) “if soluble, contain a complete determination not only of frequencies and energy values, but also of quantum-theoretical transition probabilities.” We draw attention to the strong claim here: that he has arrived at a new calculational method, which will completely determine the observable quantities. Let us now see in detail how this method works, for a harmonic oscillator perturbed by an anharmonic force of the form λx^2 per unit mass.⁴⁵

III. HEISENBERG'S CALCULATIONAL METHOD AND ITS APPLICATION TO THE ANHARMONIC OSCILLATOR

A. Recursion relations in the quantum case

The classical equation of motion is

$$\ddot{x} + \omega_0^2 x + \lambda x^2 = 0. \quad (19)$$

We depart from the order of Heisenberg's presentation and begin by showing how—as he stated—Eq. (19) leads to recursion relations for the transition amplitudes $X(n, n-\alpha)$. The $(n, n-\alpha)$ representative⁴⁶ of the first two terms in Eq. (19) is straightforward, being

$$[-\omega^2(n, n-\alpha) + \omega_0^2] X(n, n-\alpha) e^{i\omega(n, n-\alpha)t}, \quad (20)$$

while that of the third term is, by Eq. (10),

$$\lambda \sum_{\beta} X(n, n-\beta) X(n-\beta, n-\alpha) e^{i\omega(n, n-\alpha)t}. \quad (21)$$

The $(n, n-\alpha)$ representative of Eq. (19) therefore yields⁴⁷

$$[\omega_0^2 - \omega^2(n, n-\alpha)] X(n, n-\alpha) + \lambda \sum_{\beta} X(n, n-\beta) \times X(n-\beta, n-\alpha) = 0, \quad (22)$$

which generates a recursion relation for each value of α ($\alpha = 0, \pm 1, \pm 2, \dots$). For example, for $\alpha=0$ we obtain

$$\omega_0^2 X(n, n) + \lambda [X(n, n) X(n, n) + X(n, n-1) X(n-1, n) + X(n, n+1) X(n+1, n) + \dots] = 0. \quad (23)$$

No general solution for this infinite set of nonlinear algebraic equations seems to be possible, so, following Heisenberg, we turn to a perturbative approach.

B. Perturbation theory

To make the presentation self-contained, we need to discuss several ancillary results. Heisenberg began by considering the perturbative solution of the classical equation (12). He wrote the solution in the form

$$x(t) = \lambda a_0 + a_1 \cos \omega t + \lambda a_2 \cos 2\omega t + \lambda^2 a_3 \cos 3\omega t + \dots + \lambda^{\alpha-1} a_{\alpha} \cos \alpha \omega t + \dots, \quad (24)$$

where the coefficients a_{α} , and ω , are to be expanded as a power series in λ , the first terms of which are independent of λ .⁴⁸

$$a_0 = a_0^{(0)} + \lambda a_0^{(1)} + \lambda^2 a_0^{(2)} + \dots, \quad (25a)$$

$$a_1 = a_1^{(0)} + \lambda a_1^{(1)} + \lambda^2 a_1^{(2)} + \dots, \quad (25b)$$

and

$$\omega = \omega_0 + \lambda \omega^{(1)} + \lambda^2 \omega^{(2)} + \dots. \quad (26)$$

We substitute Eq. (24) into Eq. (12), use standard trigonometric identities, and equate to zero the terms that are constant and which multiply $\cos \omega t$, $\cos 2\omega t$, etc., to obtain

$$\lambda \{ \omega_0^2 a_0 + \frac{1}{2} a_1^2 + [\lambda^2 (a_0^2 + \frac{1}{2} a_2^2) + \dots] \} = 0, \quad (27a)$$

$$(-\omega^2 + \omega_0^2) a_1 + [\lambda^2 (a_1 a_2 + 2a_0 a_1) + \dots] = 0, \quad (27b)$$

$$\lambda \{ (-4\omega^2 + \omega_0^2) a_2 + \frac{1}{2} a_1^2 + [\lambda^2 (a_1 a_3 + 2a_0 a_2) + \dots] \} = 0, \quad (27c)$$

$$\lambda^2 \{ (-9\omega^2 + \omega_0^2) a_3 + a_1 a_2 + [\lambda^2 (a_1 a_4 + 2a_0 a_3) + \dots] \} = 0, \quad (27d)$$

where the dots stand for higher powers of λ . If we drop the terms of order λ^2 (and higher powers), and cancel overall factors of λ , Eq. (27) becomes (for $\lambda \neq 0$ and $a_1 \neq 0$)

$$\omega_0^2 a_0 + \frac{1}{2} a_1^2 = 0, \quad (28a)$$

$$(-\omega^2 + \omega_0^2) = 0, \quad (28b)$$

$$(-4\omega^2 + \omega_0^2) a_2 + \frac{1}{2} a_1^2 = 0, \quad (28c)$$

$$(-9\omega^2 + \omega_0^2) a_3 + a_1 a_2 = 0, \quad (28d)$$

which is the same as Eq. (H18).⁴⁹ The lowest order in λ solution is obtained from Eq. (28) by setting $\omega = \omega_0$, and replacing each a_{α} by the corresponding one with a superscript ⁽⁰⁾ [see Eq. (25)].

In the quantum case, Heisenberg proposed to seek a solution analogous to Eq. (24). Of course, it is now a matter of using the representation of $x(t)$ in terms of the quantities $X(n, n-\alpha) \exp[i\omega(n, n-\alpha)t]$. But it seems reasonable to assume that, as the index α increases from zero in integer steps, each successive amplitude will (to leading order in λ) be suppressed by an additional power of λ , as in the classical case. Thus Heisenberg suggested that, in the quantum case, $x(t)$ should be represented by terms of the form

$$\begin{aligned} &\lambda a(n, n), \quad a(n, n-1) \cos \omega(n, n-1)t, \\ &\lambda a(n, n-2) \cos \omega(n, n-2)t, \dots, \\ &\lambda^{\alpha-1} a(n, n-\alpha) \cos \omega(n, n-\alpha)t, \dots, \end{aligned} \quad (29)$$

where, as in Eqs. (25) and (26),

$$a(n, n) = a^{(0)}(n, n) + \lambda a^{(1)}(n, n) + \lambda^2 a^{(2)}(n, n) + \dots, \quad (30)$$

$$\begin{aligned} a(n, n-1) &= a^{(0)}(n, n-1) + \lambda a^{(1)}(n, n-1) \\ &\quad + \lambda^2 a^{(2)}(n, n-1) + \dots, \end{aligned} \quad (31)$$

and

$$\begin{aligned} \omega(n, n-\alpha) &= \omega^{(0)}(n, n-\alpha) + \lambda \omega^{(1)}(n, n-\alpha) \\ &\quad + \lambda^2 \omega^{(2)}(n, n-\alpha) + \dots. \end{aligned} \quad (32)$$

As Born and Jordan pointed out,⁴ some use of correspondence arguments has been made here in assuming that as $\lambda \rightarrow 0$, only transitions between adjacent states are possible. We shall return to this point in Sec. III C.

Heisenberg then simply wrote down what he asserted to be the quantum version of Eq. (28), namely⁵⁰

$$\omega_0^2 a(n, n) + \frac{1}{4} [a^2(n+1, n) + a^2(n, n-1)] = 0 \quad (33)$$

$$-\omega^2(n, n-1) + \omega_0^2 = 0, \quad (34)$$

$$\begin{aligned} [-\omega^2(n, n-2) + \omega_0^2] a(n, n-2) + \frac{1}{2} [a(n, n-1) \\ \times a(n-1, n-2)] = 0, \end{aligned} \quad (35)$$

$$\begin{aligned} [-\omega^2(n, n-3) + \omega_0^2] a(n, n-3) + \frac{1}{2} a(n, n-1) \\ \times a(n-1, n-3) + \frac{1}{2} a(n, n-2) a(n-2, n-3) = 0. \end{aligned} \quad (36)$$

The question we now address is how did Heisenberg arrive at Eqs. (33)–(36)?

We shall show that these equations can be straightforwardly derived from Eq. (22) using the ansatz (29), and we suggest that this is what Heisenberg did. This seems to be a novel proposal. Tomonaga⁸ derived Eq. (22) but then discussed only the $\lambda \rightarrow 0$ limit, that is, the simple harmonic oscillator, a special case to which we shall return in Sec. III C. The only other authors, to our knowledge, who have discussed the presumed details of Heisenberg's calculations are⁵¹ Mehra and Rechenberg.¹¹ They suggest that Heisenberg

guessed how to “translate,” “reinterpret,” or “reformulate” (their words) the classical equation (28) into the quantum ones, Eqs. (33)–(36), in a way that was consistent with his multiplication rule, Eq. (10). Although such “inspired guesswork” was undoubtedly necessary in the stages leading up to Heisenberg’s paper,¹ it seems more plausible to us that by the time of the paper’s final formulation, Heisenberg realized that he had a calculational method in which guesswork was no longer necessary, and in which Eqs. (33)–(36), in particular, could be derived.

Unfortunately, we know of no documentary evidence that directly proves (or disproves) this suggestion, but we think there is some internal evidence for it. In the passage to which attention was drawn earlier,⁴⁴ Heisenberg asserted that his formalism constituted a complete method for calculating everything that needs to be calculated. It is difficult to believe that Heisenberg did not realize that his method led directly to Eqs. (33)–(36), without the need for any “translations” of the classical relations.

To apply the ansatz of Eq. (29) to Eq. (22), we need to relate the amplitudes $X(n, n-\alpha)$ to the corresponding quantities $\lambda^{\alpha-1}a(n, n-\alpha)$. We first note that in the classical case,

$$X_\alpha(n) = X_{-\alpha}^*(n), \quad (37)$$

because $x(t)$ in Eq. (2) has to be real. Consider, without loss of generality, the case $\alpha > 0$. Then the quantum-theoretical analogue of the left-hand side of Eq. (37) is $X(n, n-\alpha)$, and that of the right-hand side is $X^*(n-\alpha, n)$ (see Ref. 27). Hence the quantum-theoretical analogue of Eq. (37) is

$$X(n, n-\alpha) = X^*(n-\alpha, n), \quad (38)$$

which is nothing but the relation $\langle n-\alpha | \hat{x} | n \rangle = \langle n | \hat{x} | n-\alpha \rangle^*$ for the Hermitian observable $\hat{x}$. Although $X(n, n-\alpha)$ can in principle be complex (and Heisenberg twice discussed the significance of the phases of such amplitudes), Heisenberg seems to have assumed (as is certainly plausible) that in the context of the classical cosine expansion in Eq. (24) and the corresponding quantum terms in Eq. (29), the $X(n, n-\alpha)$ ’s should be chosen to be real, so that Eq. (38) becomes

$$X(n, n-\alpha) = X(n-\alpha, n), \quad (39)$$

that is, the matrix with elements $\{X(n, n-\alpha)\}$ is symmetric. Consider a typical term of Eq. (29),

$$\begin{aligned} \lambda^{\alpha-1}a(n, n-\alpha)\cos[\omega(n, n-\alpha)t] \\ = \frac{\lambda^{\alpha-1}}{2}a(n, n-\alpha)[e^{i\omega(n, n-\alpha)t} + e^{-i\omega(n, n-\alpha)t}] \\ = \frac{\lambda^{\alpha-1}}{2}a(n, n-\alpha)[e^{i\omega(n, n-\alpha)t} + e^{i\omega(n-\alpha, n)t}], \end{aligned} \quad (40)$$

using $\omega(n, n-\alpha) = -\omega(n-\alpha, n)$ from Eq. (1). If we assume that $a(n, n-\alpha) = a(n-\alpha, n)$ as discussed for Eq. (39), we see that it is consistent to write

$$X(n, n-\alpha) = \frac{\lambda^{\alpha-1}}{2}a(n, n-\alpha) \quad (\alpha > 0) \quad (41)$$

and in general

$$X(n, n-\alpha) = \frac{\lambda^{|\alpha|-1}}{2}a(n, n-\alpha) \quad (\alpha \neq 0). \quad (42)$$

The case $\alpha = 0$ is clearly special, with $X(n, n) = \lambda a(n, n)$.

We may now write out the recurrence relations Eq. (22) explicitly for $\alpha = 0, 1, 2, \dots$, in terms of $a(n, n-\alpha)$ rather than $X(n, n-\alpha)$. We shall include terms up to and including terms of order λ^2 . For $\alpha = 0$ we obtain

$$\begin{aligned} \lambda\{\omega_0^2a(n, n) + \frac{1}{4}[a^2(n+1, n) + a^2(n, n-1)] + \lambda^2[a^2(n, n) \\ + \frac{1}{4}(a^2(n+2, n) + a^2(n, n-2))]\} = 0. \end{aligned} \quad (43)$$

We note the connection with Eq. (27a), and that Eq. (43) reduces to Eq. (33) when the λ^2 term is dropped and an overall factor of λ is canceled. Similarly, for $\alpha = 1$ we obtain

$$\begin{aligned} (-\omega^2(n, n-1) + \omega_0^2)a(n, n-1) + \lambda^2\{a(n, n)a(n, n-1) \\ + a(n, n-1)a(n-1, n-1) + \frac{1}{2}[a(n, n+1) \\ \times a(n+1, n-1) + a(n, n-2)a(n-2, n-1)]\} = 0 \end{aligned} \quad (44)$$

[see Eq. (27b)]. For $\alpha = 2$ we have

$$\begin{aligned} \lambda\{(-\omega^2(n, n-2) + \omega_0^2)a(n, n-2) + \frac{1}{2}a(n, n-1) \\ \times a(n-1, n-2) + \lambda^2[a(n, n)a(n, n-2) + a(n, n-2) \\ \times a(n-2, n-2) + \frac{1}{2}a(n, n+1)a(n+1, n-2) \\ + \frac{1}{2}a(n, n-3)a(n-3, n-2)]\} = 0 \end{aligned} \quad (45)$$

[see Eq. (27c)]. For $\alpha = 3$ [see Eq. (27d)] we obtain

$$\begin{aligned} \lambda^2\{(-\omega^2(n, n-3) + \omega_0^2)a(n, n-3) + \frac{1}{2}[a(n, n-1) \\ \times a(n-1, n-3) + a(n, n-2)a(n-2, n-3)] \\ + \lambda^2[a(n, n)a(n, n-3) + a(n, n-3)a(n-3, n-3) \\ + \frac{1}{2}a(n, n+1)a(n+1, n-3) + \frac{1}{2}a(n, n-4) \\ \times a(n-4, n-3)]\} = 0. \end{aligned} \quad (46)$$

If we drop the terms multiplied by λ^2 , Eqs. (43)–(46) reduce to Eqs. (33)–(36). This appears to be the first published derivation of the latter equations.

In addition to these recurrence relations which follow from the equations of motion, we also need the perturbative version of the quantum condition Eq. (16).⁵² We include terms of order λ^2 , consistent with Eqs. (43)–(46), so that Eq. (16) becomes

$$\begin{aligned} \frac{h}{\pi m} = a^2(n+1, n)\omega(n+1, n) - a^2(n, n-1)\omega(n, n-1) \\ + \lambda^2[a^2(n+2, n)\omega(n+2, n) - a^2(n, n-2) \\ \times \omega(n, n-2)]. \end{aligned} \quad (47)$$

We are now ready to obtain the solutions.

C. The lowest-order solutions for the amplitudes and frequencies

We begin by considering the lowest-order solutions in which all λ^2 terms are dropped from Eqs. (43) to (47), and all quantities (a ’s and ω ’s) are replaced by the corresponding ones with a superscript ⁽⁰⁾ [compare Eqs. (30)–(32)].⁵³ In this case, Eq. (44) reduces to

$$[-(\omega^{(0)}(n, n-1))^2 + \omega_0^2]a^{(0)}(n, n-1) = 0, \quad (48)$$

so that assuming $a^{(0)}(n, n-1) \neq 0$, we obtain

$$\omega^{(0)}(n, n-1) = \omega_0 \quad (49)$$

for all n . If we substitute Eq. (49) into the lowest-order version of Eq. (47), we find

$$\frac{h}{\pi m \omega_0} = [a^{(0)}(n+1, n)]^2 - [a^{(0)}(n, n-1)]^2. \quad (50)$$

The solution of this difference equation is

$$[a^{(0)}(n, n-1)]^2 = \frac{h}{\pi m \omega_0} (n + \text{constant}), \quad (51)$$

as given in Eq. (H20).⁵³ To determine the value of the constant, Heisenberg used the idea that in the ground state there can be no transition to a lower state. Thus

$$[a^{(0)}(0, -1)]^2 = 0, \quad (52)$$

and the constant in Eq. (51) is determined to be zero. Equation (51) then gives (up to a convention as to sign)

$$a^{(0)}(n, n-1) = \beta \sqrt{n}, \quad (53)$$

where

$$\beta = (h / \pi m \omega_0)^{1/2}. \quad (54)$$

Equations (49) and (53) were Heisenberg's first results, and they pertain to the simple (unperturbed) oscillator. We can check Eq. (53) against the usual quantum mechanical calculation via

$$a^{(0)}(n, n-1) = 2X^{(0)}(n, n-1) = 2{}_0\langle n-1 | \hat{x} | n \rangle_0, \quad (55)$$

where the states $|n\rangle_0$ are unperturbed oscillator eigenstates. It is well known that⁵⁴

$${}_0\langle n-1 | \hat{x} | n \rangle_0 = \left(\frac{\hbar}{2m\omega_0} \right)^{1/2} \sqrt{n}, \quad (56)$$

which agrees with Eq. (53), using Eq. (54). A similar treatment of Eq. (43) leads to

$$a^{(0)}(n, n) = -\frac{\beta^2}{4\omega_0^2} (2n+1). \quad (57)$$

Turning next to Eq. (45), the lowest-order form is

$$(-[\omega^{(0)}(n, n-2)]^2 + \omega_0^2) a^{(0)}(n, n-2) + \frac{1}{2} a^{(0)}(n, n-1) a^{(0)}(n-1, n-2) = 0. \quad (58)$$

Because the combination law Eq. (8) must be true for the lowest-order frequencies, we have

$$\omega^{(0)}(n, n-2) = \omega^{(0)}(n, n-1) + \omega^{(0)}(n-1, n-2) = 2\omega_0, \quad (59)$$

where we have used Eq. (49), and in general

$$\omega^{(0)}(n, n-\alpha) = \alpha\omega_0 \quad (\alpha = 1, 2, 3, \dots). \quad (60)$$

If we use Eqs. (53), (59), and (60), we obtain

$$a^{(0)}(n, n-2) = \frac{\beta^2}{6\omega_0^2} \sqrt{n(n-1)}. \quad (61)$$

A similar treatment of Eq. (46) yields

$$a^{(0)}(n, n-3) = \frac{\beta^3}{48\omega_0^4} \sqrt{n(n-1)(n-2)}. \quad (62)$$

Consideration of the lowest-order term in Eq. (22) leads to

$$a^{(0)}(n, n-\alpha) = A_\alpha \frac{\beta^\alpha}{\omega_0^{2(\alpha-1)}} \sqrt{\frac{n!}{(n-\alpha)!}}, \quad (63)$$

where A_α is a numerical factor depending on α ; Eq. (63) is equivalent to Eq. (H21).

It is instructive to comment on the relation of the above results to those that would be obtained in standard quantum-mechanical perturbation theory. At first sight, it is surprising to see nonzero amplitudes for two-quantum [Eq. (61)], three-quantum [Eq. (62)], or α -quantum [Eq. (63)] transitions appearing at lowest order. But we have to remember that in Heisenberg's perturbative ansatz, Eq. (29), the α -quantum amplitude appears multiplied by a factor $\lambda^{\alpha-1}$. Thus, for example, the lowest order two-quantum amplitude is really $\lambda a^{(0)}(n, n-2)$, not just $a^{(0)}(n, n-2)$. Indeed, such a transition is to be expected precisely at order λ^1 in conventional perturbation theory. The amplitude is $\langle n-2 | \hat{x} | n \rangle$ where, to order λ ,

$$|n\rangle = |n\rangle_0 + \frac{1}{3} m \lambda \sum_{k \neq n} \frac{{}_0\langle k | \hat{x}^3 | n \rangle_0}{(n-k)\hbar\omega_0} |k\rangle_0. \quad (64)$$

The operator $\hat{x}^3$ connects $|n\rangle_0$ to $|n+3\rangle_0, |n+1\rangle_0, |n-1\rangle_0$, and $|n-3\rangle_0$, and similar connections occur for ${}_0\langle n-2|$, so that a nonzero $O(\lambda)$ amplitude is generated in $\langle n-2 | \hat{x} | n \rangle$.

It is straightforward to check that Eq. (61) is indeed correct quantum-mechanically, but it is more tedious to check Eq. (62), and distinctly unpromising to contemplate checking Eq. (63) by doing a conventional perturbation calculation to order $\alpha-1$. For this particular problem, the improved perturbation theory represented by Eq. (29) is clearly very useful.

After having calculated the amplitudes for this problem to lowest order, Heisenberg next considered the energy. Unfortunately he again gave no details of his calculation, beyond saying that he used the classical expression for the energy, namely

$$W = \frac{1}{2} m \dot{x}^2 + \frac{1}{2} m \omega_0^2 x^2 + \frac{1}{3} m \lambda x^3. \quad (65)$$

It seems a reasonable conjecture, however, that he replaced each term in Eq. (65) by its corresponding matrix, as discussed in Sec. II A. Thus x^2 , for example, is represented by a matrix whose $(n, n-\alpha)$ element is

$$\sum_\beta X(n, n-\beta) X(n-\beta, n-\alpha) e^{i\omega(n, n-\alpha)t}, \quad (66)$$

according to his multiplication rule, Eq. (10). A similar replacement is made for x^3 , and $\dot{x}^2$ is replaced by

$$\begin{aligned} & \sum_\beta i\omega(n, n-\beta) X(n, n-\beta) e^{i\omega(n, n-\beta)t} \\ & \times i\omega(n-\beta, n-\alpha) X(n-\beta, n-\alpha) e^{i\omega(n-\beta, n-\alpha)t} \\ & = \sum_\beta \omega(n, n-\beta) \omega(n-\alpha, n-\beta) X(n, n-\beta) \\ & \times X(n-\beta, n-\alpha) e^{i\omega(n, n-\alpha)t}, \end{aligned} \quad (67)$$

using $\omega(n, m) = -\omega(m, n)$. The total energy is represented by the matrix with elements

$$W(n, n-\alpha) e^{i\omega(n, n-\alpha)t}. \quad (68)$$

It follows that if energy is to be conserved (that is, time-independent) the off-diagonal elements must vanish:

$$W(n, n - \alpha) = 0. \quad (\alpha \neq 0). \quad (69)$$

The term $\alpha = 0$ is time-independent, and may be taken to be the energy in the state n . The crucial importance of checking the condition Eq. (69) was clearly appreciated by Heisenberg.

To lowest order in λ , the last term in Eq. (65) may be dropped. Furthermore, referring to Eq. (29), the only λ -independent terms in the X -amplitudes are those involving one-quantum jumps such as $n \rightarrow n - 1$, corresponding in lowest order to amplitudes such as $X^{(0)}(n, n - 1) = \frac{1}{2}a^{(0)}(n, n - 1)$. It then follows from Eqs. (66) and (67) that the elements $W(n, n)$, $W(n, n - 2)$ and $W(n, n + 2)$, and only these elements, are independent of λ when evaluated to lowest order. In Appendix B we show that $W(n, n - 2)$ vanishes to lowest order, and $W(n, n + 2)$ vanishes similarly. Thus, to lowest order in λ , the energy is indeed conserved (as Heisenberg noted), and is given [using Eq. (66) and Eq. (67) with $\alpha = 0$ and $\beta = \pm 1$] by

$$\begin{aligned} W(n, n) &= \frac{1}{2}m[\omega^{(0)}(n, n - 1)]^2[X^{(0)}(n, n - 1)]^2 \\ &\quad + \frac{1}{2}m[\omega^{(0)}(n + 1, n)]^2[X^{(0)}(n + 1, n)]^2 \\ &\quad + \frac{1}{2}m\omega_0^2[X^{(0)}(n, n - 1)]^2 + \frac{1}{2}m\omega_0^2 \\ &\quad \times [X^{(0)}(n + 1, n)]^2 \\ &= (n + \frac{1}{2})\hbar\omega_0, \end{aligned} \quad (70)$$

where we have used Eqs. (49), (53), and (54). Equation (70) is the result given by Heisenberg in Eq. (H23).

These lowest order results are the only ones Heisenberg reported for the λx^2 term. We do not know whether he carried out higher-order calculations for this case or not. What he wrote next⁵⁵ is that 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 $\ddot{x} + \omega_0^2 + \lambda x^3 = 0$.” This case is slightly simpler because in the expression corresponding to the ansatz (29) only the odd terms are present, that is, $a_1, \lambda a_3, \lambda^2 a_5$, etc.

The results Heisenberg stated for the λx^3 problem include terms up to order λ in the amplitudes, and terms up to order λ^2 in the frequency $\omega(n, n - 1)$ and in the energy W . Once again, he gave no details of how he did the calculations. We believe there can be little doubt that he went through the algebra of solving the appropriate recurrence relations up to order λ^2 in the requisite quantities. As far as we know, the details of such a calculation have not been given before, and we believe that it is worth giving them here, as they are of both pedagogical and historical interest. In the following section we shall obtain the solutions for the λx^2 term (up to order λ^2) which we have been considering, rather than start afresh with the λx^3 term. The procedure is the same for both.

Before leaving the lowest order calculations, we address a question that may have occurred to the reader. Given that, at this stage in his paper, the main results actually relate to the simple harmonic oscillator rather than to the anharmonic one, why did Heisenberg not begin his discussion of toy models with the simplest one of all, namely the simple harmonic oscillator? And indeed, is it not possible to apply his procedure to the simple harmonic oscillator without going

through the apparent device of introducing a perturbation, and then retaining only those parts of the solution that survive as the perturbation vanishes?

For the simple harmonic oscillator, the equation of motion is $\ddot{x} + \omega_0^2 x = 0$, which yields

$$[\omega_0^2 - \omega^2(n, n - \alpha)]X(n, n - \alpha) = 0 \quad (71)$$

for the amplitudes X and frequencies ω . It is reasonable to retain the quantum condition, Eq. (16), because this condition is supposed to hold for any force law. If we assume that the only nonvanishing amplitudes are those involving adjacent states (because, for example, in the classical case only a single harmonic is present⁵⁶), then because $X(n, n - 1) = \frac{1}{2}a(n, n - 1)$, Eqs. (16) and (71) reduce to Eqs. (50) and (48), respectively, and we quickly recover our previous results. This is indeed an efficient way to solve the quantum simple harmonic oscillator.⁵⁷ For completeness, however, it would be desirable not to have to make the adjacent states assumption. Born and Jordan⁴ showed how this could be done, but their argument is somewhat involved. Soon thereafter, of course, the wave mechanics of Schrödinger and the operator approach of Dirac provided the derivations used ever since.

D. The solutions up to and including λ^2 terms

We now turn to the higher order corrections for the λx^2 term. Consider Eq. (44) and retain terms of order λ . We set [see Eqs. (25) and (26)]

$$\omega(n, n - 1) = \omega_0 + \lambda \omega^{(1)}(n, n - 1), \quad (72)$$

$$a(n, n - 1) = a^{(0)}(n, n - 1) + \lambda a^{(1)}(n, n - 1), \quad (73)$$

and find

$$2\lambda\omega_0\omega^{(1)}(n, n - 1)a^{(0)}(n, n - 1) = 0, \quad (74)$$

so that

$$\omega^{(1)}(n, n - 1) = 0. \quad (75)$$

If we consider Eq. (44) up to terms of order λ^2 and employ Eqs. (53), (57), and (61) for the zeroth-order amplitudes, we obtain the $O(\lambda^2)$ correction to $\omega(n, n - 1)$ [see Eq. (26)]:

$$\omega^{(2)}(n, n - 1) = -\frac{5\beta^2}{12\omega_0^3}n. \quad (76)$$

The corresponding corrections to $a(n, n - 1)$ are found from the quantum condition Eq. (16). To order λ we set

$$a(n + 1, n) = a^{(0)}(n + 1, n) + \lambda a^{(1)}(n + 1, n), \quad (77)$$

as in Eq. (73), and find

$$\sqrt{n + 1}a^{(1)}(n + 1, n) - \sqrt{n}a^{(1)}(n, n - 1) = 0. \quad (78)$$

Equation (78) has the solution $a^{(1)}(n, n - 1) = \text{constant}/\sqrt{n}$, but the condition $a^{(1)}(0, -1) = 0$ [see Eq. (52)] implies that the constant must be zero, and so

$$a^{(1)}(n, n - 1) = 0. \quad (79)$$

In a similar way, we obtain to order λ^2

$$\sqrt{n + 1}a^{(2)}(n + 1, n) - \sqrt{n}a^{(2)}(n, n - 1) = \frac{11\beta^3}{72\omega_0^4}(2n + 1), \quad (80)$$

which has the solution

$$a^{(2)}(n, n-1) = \frac{11\beta^3}{72\omega_0^4} n \sqrt{n}. \quad (81)$$

We now find the higher order corrections to $a(n, n)$ by considering Eq. (43). We obtain $a^{(1)}(n, n) = 0$ and

$$a^{(2)}(n, n) = -\frac{\beta^4}{72\omega_0^6} (30n^2 + 30n + 11). \quad (82)$$

Similarly, we find from Eq. (45) $a^{(1)}(n, n-2) = 0$ and

$$a^{(2)}(n, n-2) = \frac{3\beta^4}{32\omega_0^6} (2n-1) \sqrt{n(n-1)}, \quad (83)$$

where we have used

$$\begin{aligned} \omega^{(2)}(n, n-2) &= \omega^{(2)}(n, n-1) + \omega^{(2)}(n-1, n-2) \\ &= -\frac{5\beta^2}{12\omega_0^3} (2n-1). \end{aligned} \quad (84)$$

These results suffice for our purpose. If n is large, they agree with those obtained for the classical λx^2 anharmonic oscillator using the method of successive approximations.⁵⁸

As an indirect check of their quantum mechanical validity, we now turn to the energy evaluated to order λ^2 . Consider first the (n, n) element of $\frac{1}{2}m\omega_0^2\hat{x}^2$. This matrix element is given to order λ^2 , by

$$\begin{aligned} \frac{1}{2}m\omega_0^2 \left\{ \frac{1}{4} [(a^{(0)}(n, n-1))^2 + (a^{(0)}(n, n+1))^2] \right. \\ + \frac{\lambda^2}{4} [4(a^{(0)}(n, n))^2 + 2a^{(2)}(n, n-1)a^{(0)}(n-1, n) \\ + 2a^{(2)}(n, n+1)a^{(0)}(n+1, n) + (a^{(0)}(n, n-2))^2 \\ + (a^{(0)}(n, n+2))^2] \Big\} = \frac{1}{2}m\omega_0^2 \left[\frac{\beta^2}{2} \left(n + \frac{1}{2} \right) \right. \\ \left. + \frac{5\beta^4\lambda^2}{12\omega_0^4} (n^2 + n + 11/30) \right]. \end{aligned} \quad (85)$$

Similarly, using Eq. (67) up to order λ^2 , with $\alpha=0$, the (n, n) element of $\frac{1}{2}m\hat{x}^2$ is found to be

$$\frac{1}{2}m\omega_0^2 \left[\frac{\beta^2}{2} \left(n + \frac{1}{2} \right) - \frac{5\beta^4\lambda^2}{24\omega_0^4} (n^2 + n + 11/30) \right]. \quad (86)$$

Finally we consider the (n, n) element of the potential energy $\frac{1}{3}m\lambda\hat{x}^3$. To obtain the result to order λ^2 , we need to calculate the (n, n) element of $\hat{x}^3$ only to order λ . If we use

$$\begin{aligned} \hat{x}^3(n, n) &= \sum_{\alpha} \sum_{\beta} X(n, n-\alpha) X(n-\alpha, n-\beta) \\ &\quad \times X(n-\beta, n), \end{aligned} \quad (87)$$

we find that there are no zeroth-order terms, but twelve terms of order λ [recall that amplitudes such as $X(n, n)$ and $X(n, n-2)$ each carry one power of λ]. We evaluate these terms using Eqs. (53), (57), and (61), and obtain

$$-\frac{5m\lambda^2\beta^4}{24\omega_0^2} (n^2 + n + 11/30) \quad (88)$$

for this term in the energy. If we combine Eqs. (85), (86), and (88), we obtain the energy up to order λ^2 ,

$$W(n, n) = \left(n + \frac{1}{2} \right) \hbar \omega_0 - \frac{5\lambda^2\hbar^2}{12m\omega_0^4} (n^2 + n + 11/30), \quad (89)$$

a result⁵⁹ that agrees with classical perturbation theory when n is large,⁶⁰ and is in agreement with standard second-order perturbation theory in quantum mechanics.⁶¹

As mentioned, Heisenberg did not give results for the λx^2 term beyond zeroth order. He did, however, give the results for the λx^3 term up to and including λ^2 terms in the energy, and λ terms in the amplitudes. By “the energy” we mean, as usual, the (n, n) element of the energy matrix, which as noted in Sec. III C is independent of time. We also should check that the off-diagonal elements $W(n, n-\alpha)$ vanish [see Eq. (69)]. These are the terms that would (if nonzero) carry a periodic time-dependence, and Heisenberg wrote⁶² that “I could not prove in general that all periodic terms actually vanish, but this was the case for all the terms evaluated.” We do not know how many off-diagonal terms $W(n, n-\alpha)$ he evaluated, but he clearly regarded their vanishing as a crucial test of the formalism. In Appendix B we outline the calculation of all off-diagonal terms for the λx^2 term up to order λ , as an example of the kind of calculation Heisenberg probably did, finishing it late one night on Heligoland.⁶³

IV. CONCLUSION

We have tried to remove some of the barriers to understanding Heisenberg’s 1925 paper by providing the details of calculations of the type we believe he performed. We hope that more people will thereby be encouraged to appreciate this remarkable paper.

The fact is that Heisenberg’s “amplitude calculus” works, at least for the simple one-dimensional problems to which he applied it. It is an eminently practical procedure, requiring no sophisticated mathematical knowledge to implement. Because it uses the correct equations of motion and incorporates the fundamental commutator, Eq. (11), via the quantum condition, Eq. (16), the answers obtained are correct, in agreement with conventional quantum mechanics.

We believe that Heisenberg’s approach, as applied to simple dynamical systems, has much pedagogical value, and could usefully be included in undergraduate courses on quantum mechanics. The multiplication rule, Eq. (10), has a convincing physical rationale, even for those who (like Heisenberg) do not recognize it as matrix multiplication. Indeed, this piece of quantum physics could provide an exciting application for those learning about matrices in a concurrent mathematics course. The simple examples of Eq. (10), in equations such as Eq. (22) or the analogous one for the $\lambda\hat{x}^3$ term, introduce students directly to the fundamental quantum idea that a transition from one state to another occurs via all possible intermediate states, something that can take time to emerge in the traditional wave-mechanical approach. The solution of the quantum simple harmonic oscillator, sketched at the end of Sec III D, is simple in comparison with the standard methods. Finally, the type of perturbation theory employed here provides an instructive introduction to the technique, being more easily related to the classical analysis than is conventional quantum-mechanical perturbation theory (which students tend to find very formal).

It is true that many important problems in quantum mechanics are much more conveniently handled in the wave-mechanical formalism: unbound problems are an obvious example, but even the Coulomb problem required a famous *tour de force* by Pauli.⁶⁴ Nevertheless, a useful seed may be sown, so that when students meet problems involving a finite number of discrete states—for example, in the treatment of spin—the introduction of matrices will come as less of a shock. And they may enjoy the realization that the somewhat mysteriously named “matrix elements” of wave mechanics are indeed the elements of Heisenberg’s matrices.

APPENDIX A: THE QUANTUM CONDITION, EQ. (16), AND $\hat{x}\hat{p}-\hat{p}\hat{x}=i\hbar$

Consider the (n,n) element of $(\hat{x}\hat{\dot{x}}-\hat{\dot{x}}\hat{x})$, which is

$$\sum_{\alpha} X(n,n-\alpha) i\omega(n-\alpha,n) X(n-\alpha,n) - \sum_{\alpha} i\omega(n,n-\alpha) X(n,n-\alpha) X(n-\alpha,n). \quad (\text{A1})$$

In the first term of Eq. (A1), the sum over $\alpha>0$ may be rewritten as

$$-i \sum_{\alpha>0} \omega(n,n-\alpha) |X(n,n-\alpha)|^2 \quad (\text{A2})$$

using $\omega(n,n-\alpha)=-\omega(n-\alpha,n)$ from Eq. (1) and $X(n-\alpha,n)=X^*(n,n-\alpha)$ from Eq. (38). Similarly, the sum over $\alpha<0$ becomes

$$i \sum_{\alpha>0} \omega(n+\alpha,n) |X(n+\alpha,n)|^2 \quad (\text{A3})$$

on changing α to $-\alpha$. Similar steps for the second term of Eq. (A1) lead to the result

$$\begin{aligned} (\hat{x}\hat{\dot{x}}-\hat{\dot{x}}\hat{x})(n,n) &= 2i \sum_{\alpha>0} [\omega(n+\alpha,n) |X(n+\alpha,n)|^2 \\ &\quad - \omega(n,n-\alpha) |X(n,n-\alpha)|^2] \\ &= 2i\hbar/(4\pi m), \end{aligned} \quad (\text{A4})$$

where the last step follows from Eq. (16). We set $\hat{p}=m\hat{\dot{x}}$ and find

$$(\hat{x}\hat{p}-\hat{p}\hat{x})(n,n)=i\hbar \quad (\text{A5})$$

for all values of n . Equation (A5) was found by Born⁴³ shortly after reading Heisenberg’s paper. In further developments the value of the fundamental commutator $\hat{x}\hat{p}-\hat{p}\hat{x}$, namely $i\hbar$, was taken to be a basic postulate. The sum rule in Eq. (16) is then derived by taking the (n,n) matrix element of the relation $[\hat{x},[\hat{H},\hat{x}]]=\hbar^2/m$.

APPENDIX B: CALCULATION OF THE OFF-DIAGONAL MATRIX ELEMENTS OF THE ENERGY $W(n,n-\alpha)$ FOR THE λx^2 TERM

We shall show that, for $\alpha\neq 0$, all the elements $(n,n-\alpha)$ of the energy operator $\frac{1}{2}m\hat{\dot{x}}^2 + \frac{1}{2}m\omega_0^2\hat{x}^2 + \frac{1}{3}\lambda m\hat{x}^3$ vanish up to order λ . We begin by noting that at any given order in λ , only a limited number of elements $W(n,n-1), W(n,n-2), \dots$

will contribute, because the amplitudes $X(n,n-\alpha)$ are suppressed by increasing powers of λ as α increases. In fact, for $\alpha\geq 2$ the leading power of λ in $W(n,n-\alpha)$ is $\lambda^{\alpha-2}$, which arises from terms such as $X(n,n-1)X(n-1,n-\alpha)$ and $\lambda X(n,n-1)X(n-1,n-2)X(n-2,n-\alpha)$. Thus to order λ , we need to calculate only $W(n,n-1), W(n,n-2), W(n,n-3)$.

(a) $W(n,n-1)$. There are four $O(\lambda)$ contributions to the $(n,n-1)$ element of $\frac{1}{2}m\omega_0^2\hat{x}^2$:

$$\begin{aligned} \frac{1}{4}m\omega_0^2\lambda\{a^{(0)}(n,n)a^{(0)}(n,n-1)+a^{(0)}(n,n-1) \\ \times a^{(0)}(n-1,n-1)+\frac{1}{2}[a^{(0)}(n,n+1)a^{(0)}(n+1,n-1) \\ +a^{(0)}(n,n-2)a^{(0)}(n-2,n-1)]\} \\ = -\frac{5}{24}m\lambda\beta^3n\sqrt{n}. \end{aligned} \quad (\text{B1})$$

There are two $O(\lambda)$ contributions to the $(n,n-1)$ element of $\frac{1}{2}m\hat{x}^2$:

$$\begin{aligned} -\frac{1}{8}\lambda m\{\omega^{(0)}(n,n+1)\omega^{(0)}(n+1,n-1)a^{(0)}(n,n+1) \\ \times a^{(0)}(n+1,n-1)+\omega^{(0)}(n,n-2)\omega^{(0)}(n-2,n-1) \\ \times a^{(0)}(n,n-2)a^{(0)}(n-2,n-1)\} = \frac{1}{12}m\lambda\beta^3n\sqrt{n}. \end{aligned} \quad (\text{B2})$$

There are three $O(\lambda)$ contributions to the $(n,n-1)$ element of $\frac{1}{3}\lambda m\hat{x}^3$:

$$\begin{aligned} \frac{1}{24}m\lambda\{a^{(0)}(n,n-1)a^{(0)}(n-1,n)a^{(0)}(n,n-1) \\ +a^{(0)}(n,n-1)a^{(0)}(n-1,n-2)a^{(0)}(n-2,n-1) \\ +a^{(0)}(n,n+1)a^{(0)}(n+1,n)a^{(0)}(n,n-1)\} \\ = \frac{1}{8}m\lambda\beta^3n\sqrt{n}. \end{aligned} \quad (\text{B3})$$

The sum of Eqs. (B1)–(B3) vanishes, as required.

(b) $W(n,n-2)$. The leading contribution is independent of λ . From the term $\frac{1}{2}m\omega_0^2\hat{x}^2$, it is

$$\frac{1}{8}m\omega_0^2a^{(0)}(n,n-1)a^{(0)}(n-1,n-2), \quad (\text{B4})$$

which is canceled by the corresponding term from $\frac{1}{2}m\hat{x}^2$. The next terms are $O(\lambda^2)$, for example from the leading term in the $(n,n-2)$ element of $\frac{1}{3}\lambda m\hat{x}^3$.

(c) $W(n,n-3)$. There are two $O(\lambda)$ contributions from $\frac{1}{2}m\omega_0^2\hat{x}^2$:

$$\begin{aligned} \frac{1}{8}m\omega_0^2\lambda\{a^{(0)}(n,n-1)a^{(0)}(n-1,n-3) \\ +a^{(0)}(n,n-2)a^{(0)}(n-2,n-3)\} \\ = \frac{1}{24}m\lambda\beta^3\sqrt{n(n-1)(n-2)}. \end{aligned} \quad (\text{B5})$$

There are two $O(\lambda)$ contributions from $\frac{1}{2}m\hat{x}^2$:

$$\begin{aligned} -\frac{1}{8}m\lambda\{\omega^{(0)}(n,n-1)a^{(0)}(n,n-1)\omega^{(0)}(n-1,n-3) \\ \times a^{(0)}(n-1,n-3)+\omega^{(0)}(n,n-2) \\ \times a^{(0)}(n,n-2)\omega^{(0)}(n-2,n-3)a^{(0)}(n-2,n-3)\} \\ = -\frac{1}{12}\lambda m\beta^3\sqrt{n(n-1)(n-2)}. \end{aligned} \quad (\text{B6})$$

There is only one $O(\lambda)$ contribution from $\frac{1}{3}\lambda m\hat{x}^3$:

$$\begin{aligned} & \frac{1}{24} m \lambda a^{(0)}(n, n-1) a^{(0)}(n-1, n-2) a^{(0)}(n-2, n-3) \\ &= \frac{1}{24} \lambda m \beta^3 \sqrt{n(n-1)(n-2)}. \end{aligned} \quad (\text{B7})$$

The sum of Eqs. (B5)–(B7) vanishes, as required.

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¹W. Heisenberg, “Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen,” *Z. Phys.* **33**, 879–893 (1925).

²This is the title of the English translation, which is paper 12 in Ref. 3, pp. 261–276. We shall refer exclusively to this translation, and to the equations in it as (H1), (H2), ...

³*Sources of Quantum Mechanics*, edited by B. L. van der Waerden (North-Holland, Amsterdam, 1967). A collection of reprints in translation.

⁴M. Born and P. Jordan, “Zur Quantenmechanik,” *Z. Phys.* **34**, 858–888 (1925), paper 13 in Ref. 3.

⁵P. A. M. Dirac, “The fundamental equations of quantum mechanics,” *Proc. R. Soc. London, Ser. A* **109**, 642–653 (1926), paper 14 in Ref. 3.

⁶M. Born, W. Heisenberg, and P. Jordan, “Zur Quantenmechanik II,” *Z. Phys.* **35**, 557–615 (1926), paper 15 in Ref. 3.

⁷S. Weinberg, *Dreams of a Final Theory* (Pantheon, New York, 1992), pp. 53–54. Weinberg goes on to say that “Perhaps we should not look too closely at Heisenberg’s first paper ...” We will not follow his suggestion here.

⁸S.-I. Tomonaga, *Quantum Mechanics: Old Quantum Theory* (North-Holland, Amsterdam, 1962), Vol. 1.

⁹M. Jammer, *The Conceptual Development of Quantum Mechanics* (McGraw-Hill, New York, 1966).

¹⁰E. MacKinnon, “Heisenberg, models and the rise of matrix mechanics,” *Hist. Stud. Phys. Sci.* **8**, 137–188 (1977).

¹¹J. Mehra and H. Rechenberg, *The Historical Development of Quantum Theory* (Springer-Verlag, New York, 1982), Vol. 2.

¹²J. Hendry, *The Creation of Quantum Mechanics and the Bohr-Pauli Dialogue* (Reidel, Dordrecht, 1984).

¹³T.-Y. Wu, *Quantum Mechanics* (World Scientific, Singapore, 1986).

¹⁴M. Taketani and M. Nagasaki, *The Formation and Logic of Quantum Mechanics* (World Scientific, Singapore, 2002), Vol. 3.

¹⁵G. Birtwistle, *The New Quantum Mechanics* (Cambridge U.P., Cambridge, 1928).

¹⁶M. Born, *Atomic Physics* (Dover, New York, 1989).

¹⁷J. Lacki, “Observability, Anschaulichkeit and abstraction: A journey into Werner Heisenberg’s science and philosophy,” *Fortschr. Phys.* **50**, 440–458 (2002).

¹⁸J. Mehra, *The Golden Age of Theoretical Physics* (World Scientific, Singapore, 2001), Vol. 2.

¹⁹Of these the most detailed are Ref. 3, pp. 28–35, Ref. 8, pp. 204–224, Ref. 10, pp. 161–188, and Ref. 11, Chap. IV.

²⁰Reference 7, p. 53.

²¹Reference 2, p. 262.

²²All quotations are from the English translation of Ref. 2.

²³We use ω rather than Heisenberg’s ν .

²⁴We depart from the notation of Refs. 1 and 2, preferring that of Ref. 8, pp. 204–224. Our $X_\alpha(n)$ is Heisenberg’s $a_\alpha(n)$.

²⁵The reader may find it helpful at this point to consult Ref. 26, which provides a clear account of the connection between the classical analysis of an electron’s periodic motion and simple quantum versions. See also J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1975), 2nd ed., Sec. 9.2.

²⁶W. A. Fedak and J. J. Prentis, “Quantum jumps and classical harmonics,” *Am. J. Phys.* **70**, 332–344 (2002).

²⁷The association $X_\alpha(n) \leftrightarrow X(n, n-\alpha)$ is generally true only for non-negative α . For negative values of α , a general term in the classical Fourier series is $X_{-|\alpha|}(n) \exp[-i\omega(n)|\alpha|t]$. If we replace $-\omega(n)|\alpha|$ by $-\omega(n, n-|\alpha|)$, which is equal to $\omega(n-|\alpha|, n)$ using Eq. (1), we see that $X_{-|\alpha|}(n) \leftrightarrow X(n-|\alpha|, n)$. The association $X_{-|\alpha|} \leftrightarrow X(n, n+|\alpha|)$ would not be correct because $\omega(n, n+|\alpha|)$ is not the same, in general, as $\omega(n-|\alpha|, n)$.

²⁸Conventional notation, subsequent to Ref. 4, would replace $n-\alpha$ by a second index m , say. We prefer to remain as close as possible to the notation of Heisenberg’s paper.

²⁹Reference 2, p. 264.

³⁰Reference 2, p. 265.

³¹Reference 2, p. 266.

³²Reference 2 p. 267.

³³This step apparently did not occur to him immediately. See Ref. 11, p. 231.

³⁴Actually not quite. We have taken the liberty of changing the order of the arguments in the first terms in the braces; this (correct) order is as given in the equation Heisenberg wrote before Eq. (H20).

³⁵W. Thomas, “Über die Zahl der Dispersionselektronen, die einem stationären Zustände zugeordnet sind (Vorläufige Mitteilung),” *Naturwissenschaften* **13**, 627 (1925).

³⁶W. Kuhn, “Über die Gesamtstärke der von einem Zustande ausgehenden Absorptionslinien,” *Z. Phys.* **33**, 408–412 (1925), paper 11 in Ref. 3.

³⁷W. Heisenberg, as discussed in Ref. 11, pp. 243 ff.

³⁸Reference 9, p. 193; Φ is any function defined for stationary states.

³⁹M. Born, “Über Quantenmechanik,” *Z. Phys.* **26**, 379–395 (1924), paper 7 in Ref. 3.

⁴⁰Reference 9, p. 202.

⁴¹H. A. Kramers and W. Heisenberg, “Über die Streuung von Strahlen durch Atome,” *Z. Phys.* **31**, 681–707 (1925), paper 10 in Ref. 3.

⁴²For considerable further detail on dispersion theory, sum rules, and the “discretization” rules, see Ref. 8, pp. 142–147, 206–208, and Ref. 9, Sec. 4.3.

⁴³See Ref. 3, p. 37.

⁴⁴Reference 2, p. 268.

⁴⁵For an interesting discussion of the possible reasons why he chose to try out his method on the anharmonic oscillator, see Ref. 11, pp. 232–235; and Ref. 3, p. 22. Curiously, most of the commentators—with the notable exception of Tomonaga (Ref. 8)—seem to lose interest in the details of the calculations at this point.

⁴⁶The $(n, n-\alpha)$ matrix element, in the standard terminology.

⁴⁷Equation (22) is not in Heisenberg’s paper, although it is given by Tomonaga, Ref. 8, Eq. (32.20’).

⁴⁸Note that this means that, in $x(t)$, all the terms which are of order λ^p arise from many different terms in Eq. (24).

⁴⁹Except that Heisenberg relabeled most of the a_α ’s as $a_\alpha(n)$.

⁵⁰Because of an oversight, he wrote $a_0(n)$ in place of $a(n, n)$ in Eq. (33).

⁵¹MacKinnon (Ref. 10) suggests how, in terms of concepts from the “virtual oscillator” model, Eq. (28) may be transformed into Eqs. (33)–(36). We do not agree with MacKinnon (Ref. 10, footnote 62) regarding “mistakes” in Eqs. (35) and (36).

⁵²In the version of the quantum condition that Heisenberg gave just before Eq. (H20), he unfortunately used the same symbol for the transition amplitudes as in (H16)—see Eq. (16)—but replaced $4\pi m$ by πm , not explaining where the factor 1/4 came from [see Eq. (42)]; he also omitted the λ ’s.

⁵³Heisenberg omitted the superscripts.

⁵⁴See, for example, L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1968), 3rd ed., p. 72.

⁵⁵Reference 2, p. 272.

⁵⁶This is the justification suggested in Ref. 4, p. 297 of paper 13 in Ref. 3.

⁵⁷It is essentially that given by L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, Oxford, 1977), 3rd ed., pp. 67–68.

⁵⁸L. D. Landau and E. M. Lifshitz, *Mechanics* (Pergamon, Oxford, 1976), 3rd ed., pp. 86–87.

⁵⁹This equation corresponds to Eq. (88) of Ref. 4, in which there appears to be a misprint of 17/30 instead of 11/30.

⁶⁰See Ref. 4, p. 305.

⁶¹Reference 57, p. 136.

⁶²Reference 2, pp. 272–3.

⁶³See W. Heisenberg, *Physics and Beyond* (Allen & Unwin, London, 1971), p. 61.

⁶⁴W. Pauli, “Über das Wasserstoffspektrum vom Standpunkt der neuen Quantenmechanik,” *Z. Phys.* **36**, 336–363 (1926), paper 16 in Ref. 3.