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

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 papers[2] 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

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

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

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[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

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

and in classical theory of the form

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

(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:

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

Quantum-theoretical:

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

or

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

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:

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

Classical:

$$\mathrm{Re}\{\mathfrak{A}_\alpha(n)\; e^{i\omega(n)\alpha t}\}. \tag{2}$$

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 $x(t)$:

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

or

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

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

The answer in classical theory is obviously:

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

or

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

so that

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

or, respectively,

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

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

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

or

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

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:

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

Quantum-theoretical:

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

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

or the corresponding integral forms.

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[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 represen-tation 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 quanti-ties $x(t)$, $y(t)$, 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 kine-matics of quantum theory, we turn our attention to the dynamical problem which aims at the determination of the $\mathfrak{A}$, v, W from the given forces of the system. In earlier theory this problem was solved in two stages:

1. Integration of the equation of motion

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

2. Determination of the constants for periodic motion through

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

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:

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

hence

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

and

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

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

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

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

$$\frac{\mathrm{d}}{\mathrm{d}n}(nh) = \frac{\mathrm{d}}{\mathrm{d}n}\oint m\dot{x}^2\,\mathrm{d}t,$$

that is,

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

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]

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

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

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[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 $\frac{1}{2}m\dot{x}^2+U(x)=$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 $E\cos 2\pi\nu t$:

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

$$\left. - \frac{|a(n, n-\alpha)|^2\nu(n, n-\alpha)}{\nu^2(n, n-\alpha)-\nu^2} \right\},$$

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:

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

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

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

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:

$$\omega_0^2 a_0(n) + \tfrac{1}{2} a_1^2(n) = 0;$$
$$- \omega^2 + \omega_0^2 = 0;$$
$$(- 4\omega^2 + \omega_0^2)a_2(n) + \tfrac{1}{2} a_1^2 = 0; \tag{18}$$
$$(- 9\omega^2 + \omega_0^2)a_3(n) + a_1 a_2 = 0;$$

$$\cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot$$

Quantum-theoretical:

$$\omega_0^2 a_0(n) + \tfrac{1}{4}[a^2(n + 1, n) + a^2(n, n - 1)] = 0;$$
$$- \omega^2(n, n - 1) + \omega_0^2 = 0;$$
$$[-\omega^2(n, n-2)+\omega_0^2]a(n, n-2)+\tfrac{1}{2}[a(n, n-1)a(n-1, n-2)] = 0; \tag{19}$$
$$[- \omega^2(n, n - 3) + \omega_0^2]a(n, n - 3)$$
$$+\tfrac{1}{2}[a(n, n-1)a(n-1, n-3)]+\tfrac{1}{2}[a(n, n-2)a(n-2, n-3)] = 0;$$

$$\cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot$$

The additional quantum condition is:
Classical $(J=nh)$:

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

Quantum-theoretical:

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

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

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

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

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

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

where $\varkappa(\tau)$ 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 $\tfrac{1}{2}m\dot{x}^2+\tfrac{1}{2}m\omega_0^2 x^2+\tfrac{1}{3}m\lambda x^3=W$, because in the present first-approximation calculation it actually is constant, even when treated quantum-theoretically. Its value is given by (19), (20) and (21) as:

Classical:

$$W = nh\omega_0/2\pi. \tag{22}$$

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

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

(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

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

quantum-theoretically we attempt to set by analogy

$$a(n, n-1) \cos \omega(n, n-1)t; \qquad \lambda a(n, n-3) \cos \omega(n, n-3)t; \qquad \ldots$$

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

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

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

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

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

$$a(n, n-3) = \frac{1}{32} \sqrt{\frac{h^3}{\pi^3\omega_0^7 m^3}} \, n(n-1)(n-2) \cdot$$

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

The energy, defined as the constant term in the expression

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

(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

$$W = \frac{(n + \frac{1}{2})h\omega_0}{2\pi} + \lambda \, \frac{3(n^2 + n + \frac{1}{2})h^2}{8 \cdot 4\pi^2\omega_0^2 m}$$

$$- \lambda^2 \, \frac{h^3}{512\pi^3\omega_0^5 m^2} \, (17n^3 + \tfrac{51}{2}n^2 + \tfrac{59}{2}n + \tfrac{21}{2}). \quad (27)$$

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 effect[1] 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),

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

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

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

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

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

The energy is

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

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

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

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 $\mathfrak{o}$ 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

$$z: \quad a(n, n-1; m, m) \cos \omega(n, n-1)t;$$

$$x + iy: \quad b(n, n-1; m, m-1) e^{i[\omega(n, n-1)+\mathfrak{o}]t};$$

$$b(n, n-1; m-1, m) e^{i[-\omega(n, n-1)+\mathfrak{o}]t}.$$

The equations of motion are simply

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

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

Because of (7) this leads to[1]

$$\tfrac{1}{2}\{\tfrac{1}{2}a^2(n, n-1; m, m)+b^2(n, n-1; m, m-1)+b^2(n, n-1; m, m+1)$$
$$+ \tfrac{1}{2}a^2(n+1, n; m, m) + b^2(n+1, n; m-1, m)$$
$$+ b^2(n+1, n; m+1, m)\} = a^2. \tag{30}$$

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

One also has the quantum condition from (16):

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

The classical relations corresponding to these equations are

$$\tfrac{1}{2}a_0^2 + b_1^2 + b_{-1}^2 = a^2;$$
$$\tfrac{1}{4}a_0^2 = b_1 b_{-1}; \tag{33}$$
$$2\pi m(b_{+1}^2 - b_{-1}^2)\omega = (m + \text{const})h.$$

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:

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

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

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

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

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[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 1925[1] 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, Weinberg[7] 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, MacKinnon[10] and Mehra and Rechenberg[11] 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 frequencies[23]

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

and noted that these frequencies, which characterize the radiation emitted in the transition $n \to n - \alpha$, 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

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

where α is an integer.[24] According to classical theory, the energy emitted per unit time (the power) in a transition corresponding to the αth harmonic $\alpha\omega(n)$ is[25]

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

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

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

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 wrote[29] 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

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

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

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

where

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

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:

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

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 words[30]) to combine the quantum amplitudes in such a way as to ensure the frequency combination Eq. (8), that is, as

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

or

$$Y(n,n-\beta) = \sum_\alpha X(n,n-\alpha)X(n-\alpha,n-\beta), \qquad (10)$$

which is Heisenberg's rule for multiplying transition amplitudes. Note particularly that the replacements $X_\alpha(n) \to X(n,n-\alpha)$, 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 once[31] 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 noncommutativity (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 paper[4] to state the fundamental commutation relation (in modern notation)

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

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

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

and by determining the constants of the periodic motion through the ''quantum condition''

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

where the integral is evaluated over one period. In regard to Eq. (12), Heisenberg wrote[32] 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 that[32] ''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

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

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)]

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

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

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

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 Jammer[38] calls Born's correspondence rule, namely[39]

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

or rather to its iteration to the form[40]

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

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 guess[43] 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 noted[44] 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 statement[44] 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

$$\ddot{x}+\omega_0^2 x+\lambda x^2=0. \tag{19}$$

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 $(n,n-\alpha)$ representative[46] of the first two terms in Eq. (19) is straightforward, being

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

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 yields[47]

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

$$\times X(n-\beta,n-\alpha)=0, \quad (22)$$

which generates a recursion relation for each value of α ($\alpha=0,\pm1,\pm2,...$). For example, for $\alpha=0$ we obtain

$$\omega_0^2 X(n,n)+\lambda[X(n,n)X(n,n)+X(n,n-1)X(n-1,n)$$

$$+X(n,n+1)X(n+1,n)+\cdots]=0. \quad (23)$$

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

$$x(t)=\lambda a_0+a_1\cos\omega t+\lambda a_2\cos2\omega t+\lambda^2 a_3\cos3\omega t$$

$$+\cdots+\lambda^{\alpha-1}a_\alpha\cos\alpha\omega t+\cdots, \quad (24)$$

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]

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

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

and

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

We substitute Eq. (24) into Eq. (12), use standard trigonometric identities, and equate to zero the terms that are constant and which multiply $\cos\omega t$, $\cos2\omega t$, etc., to obtain

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

$$(-\omega^2+\omega_0^2)a_1+[\lambda^2(a_1a_2+2a_0a_1)+\cdots]=0, \quad (27b)$$

$$\lambda\{(-4\omega^2+\omega_0^2)a_2+\tfrac{1}{2}a_1^2+[\lambda^2(a_1a_3+2a_0a_2)+\cdots]\}$$

$$=0, \quad (27c)$$

$$\lambda^2\{(-9\omega^2+\omega_0^2)a_3+a_1a_2+[\lambda^2(a_1a_4+2a_0a_3)+\cdots]\}$$

$$=0, \quad (27d)$$

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 $\lambda\neq0$ and $a_1\neq0$)

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

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

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

$$(-9\omega^2+\omega_0^2)a_3+a_1a_2=0, \quad (28d)$$

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

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

$$\lambda a(n,n-2)\cos\omega(n,n-2)t,...,$$

$$\lambda^{\alpha-1}a(n,n-\alpha)\cos\omega(n,n-\alpha)t,..., \quad (29)$$

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

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

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

$$+\lambda^2 a^{(2)}(n,n-1)+\cdots, \quad (31)$$

and

$$\omega(n,n-\alpha)=\omega^{(0)}(n,n-\alpha)+\lambda\omega^{(1)}(n,n-\alpha)$$

$$+\lambda^2\omega^{(2)}(n,n-\alpha)+\cdots. \quad (32)$$

As Born and Jordan pointed out,[4] some use of correspondence arguments has been made here in assuming that as $\lambda\rightarrow0$, 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), namely[50]

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

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

$$[-\omega^2(n,n-2)+\omega_0^2]a(n,n-2)+\tfrac{1}{2}[a(n,n-1)$$

$$\times a(n-1,n-2)]=0, \quad (35)$$

$$[-\omega^2(n,n-3)+\omega_0^2]a(n,n-3)+\tfrac{1}{2}a(n,n-1)$$

$$\times a(n-1,n-3)+\tfrac{1}{2}a(n,n-2)a(n-2,n-3)=0. \quad (36)$$

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. Tomonaga[8] derived Eq. (22) but then discussed only the $\lambda\rightarrow0$ 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 are[51] 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,

$$X_\alpha(n)=X^*_{-\alpha}(n),\tag{37}$$

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

$$X(n,n-\alpha)=X^*(n-\alpha,n),\tag{38}$$

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

$$X(n,n-\alpha)=X(n-\alpha,n),\tag{39}$$

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

$$\lambda^{\alpha-1}a(n,n-\alpha)\cos[\omega(n,n-\alpha)t]$$

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

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

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

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

and in general

$$X(n,n-\alpha)=\frac{\lambda^{|\alpha|-1}}{2}a(n,n-\alpha)\quad(\alpha\neq0).\tag{42}$$

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 $\alpha=0,1,2,\ldots$, 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

$$\lambda\{\omega_0^2a(n,n)+\tfrac{1}{4}[a^2(n+1,n)+a^2(n,n-1)]+\lambda^2[a^2(n,n)$$

$$+\tfrac{1}{4}(a^2(n+2,n)+a^2(n,n-2))]\}=0.\tag{43}$$

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

$$(-\omega^2(n,n-1)+\omega_0^2)a(n,n-1)+\lambda^2\{a(n,n)a(n,n-1)$$

$$+a(n,n-1)a(n-1,n-1)+\tfrac{1}{2}[a(n,n+1)$$

$$\times a(n+1,n-1)+a(n,n-2)a(n-2,n-1)]\}=0\tag{44}$$

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

$$\lambda\{(-\omega^2(n,n-2)+\omega_0^2)a(n,n-2)+\tfrac{1}{2}a(n,n-1)$$

$$\times a(n-1,n-2)+\lambda^2[a(n,n)a(n,n-2)+a(n,n-2)$$

$$\times a(n-2,n-2)+\tfrac{1}{2}a(n,n+1)a(n+1,n-2)$$

$$+\tfrac{1}{2}a(n,n-3)a(n-3,n-2)]\}=0\tag{45}$$

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

$$\lambda^2\{(-\omega^2(n,n-3)+\omega_0^2)a(n,n-3)+\tfrac{1}{2}[a(n,n-1)$$

$$\times a(n-1,n-3)+a(n,n-2)a(n-2,n-3)]$$

$$+\lambda^2[a(n,n)a(n,n-3)+a(n,n-3)a(n-3,n-3)$$

$$+\tfrac{1}{2}a(n,n+1)a(n+1,n-3)+\tfrac{1}{2}a(n,n-4)$$

$$\times a(n-4,n-3)]\}=0.\tag{46}$$

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

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

$$+\lambda^2[a^2(n+2,n)\omega(n+2,n)-a^2(n,n-2)$$

$$\times\omega(n,n-2)].\tag{47}$$

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

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

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

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

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

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

The solution of this difference equation is

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

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

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

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

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

where

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

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

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

where the states $|n\rangle_0$ are unperturbed oscillator eigenstates. It is well known that[54]

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

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

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

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

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

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

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

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

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

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

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

A similar treatment of Eq. (46) yields

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

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

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

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,

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

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

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

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

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

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

$$\sum_\beta i\omega(n,n-\beta)X(n,n-\beta)e^{i\omega(n,n-\beta)t}$$
$$\times i\omega(n-\beta,n-\alpha)X(n-\beta,n-\alpha)e^{i\omega(n-\beta,n-\alpha)t}$$
$$=\sum_\beta \omega(n,n-\beta)\omega(n-\alpha,n-\beta)X(n,n-\beta)$$
$$\times X(n-\beta,n-\alpha)e^{i\omega(n,n-\alpha)t}, \qquad (67)$$

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

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

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

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

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 $n\to n-1$, 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

$$W(n,n)=\frac{1}{2}m[\omega^{(0)}(n,n-1)]^2[X^{(0)}(n,n-1)]^2$$
$$+\frac{1}{2}m[\omega^{(0)}(n+1,n)]^2[X^{(0)}(n+1,n)]^2$$
$$+\frac{1}{2}m\omega_0^2[X^{(0)}(n,n-1)]^2+\frac{1}{2}m\omega_0^2$$
$$\times[X^{(0)}(n+1,n)]^2$$
$$=(n+\tfrac{1}{2})\hbar\omega_0, \qquad (70)$$

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 next[55] 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

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

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 present[56]), 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 Jordan[4] 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)]

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

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

and find

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

so that

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

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)]:

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

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

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

as in Eq. (73), and find

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

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

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

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

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

which has the solution

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

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

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

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

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

where we have used

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

$$= -\frac{5\beta^2}{12\omega_0^3}(2n-1). \qquad (84)$$

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

$$\frac{1}{2}m\omega_0^2 \left\{ \frac{1}{4}[(a^{(0)}(n,n-1))^2 + (a^{(0)}(n,n+1))^2] \right.$$

$$+ \frac{\lambda^2}{4}[4(a^{(0)}(n,n))^2 + 2a^{(2)}(n,n-1)a^{(0)}(n-1,n)$$

$$+ 2a^{(2)}(n,n+1)a^{(0)}(n+1,n) + (a^{(0)}(n,n-2))^2$$

$$\left. + (a^{(0)}(n,n+2))^2] \right\} = \frac{1}{2}m\omega_0^2 \left[\frac{\beta^2}{2}\left(n+\frac{1}{2}\right) \right.$$

$$\left. + \frac{5\beta^4\lambda^2}{12\omega_0^4}(n^2 + n + 11/30) \right]. \qquad (85)$$

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

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

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

$$\hat{x}^3(n,n) = \sum_\alpha \sum_\beta X(n, n-\alpha)X(n-\alpha, n-\beta)$$

$$\times X(n-\beta, n), \qquad (87)$$

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

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

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

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

a result[59] 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 wrote[62] 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 $(\hat{x}\dot{\hat{x}}-\dot{\hat{x}}\hat{x})$, which is

$$\sum_{\alpha} X(n,n-\alpha)i\omega(n-\alpha,n)X(n-\alpha,n)$$

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

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

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

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

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

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

$$(\hat{x}\dot{\hat{x}}-\dot{\hat{x}}\hat{x})(n,n)=2i\sum_{\alpha>0} [\omega(n+\alpha,n)|X(n+\alpha,n)|^2$$

$$-\omega(n,n-\alpha)|X(n,n-\alpha)|^2]$$

$$=2ih/(4\pi m), \quad (A4)$$

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

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

for all values of n. Equation (A5) was found by Born[43] 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 $\alpha\neq0$, all the elements $(n,n-\alpha)$ of the energy operator $\frac{1}{2}m\dot{\hat{x}}^2+\frac{1}{2}m\omega_0^2\hat{x}^2+\frac{1}{3}\lambda m\hat{x}^3$ vanish up to order λ. We begin by noting that at any given order in λ, only a limited number of elements $W(n,n-1),W(n,n-2),\ldots$

will contribute, because the amplitudes $X(n,n-\alpha)$ are suppressed by increasing powers of λ as α increases. In fact, for $\alpha\geq2$ 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 $\frac{1}{2}m\omega_0^2\hat{x}^2$:

$$\frac{1}{4}m\omega_0^2\lambda\{a^{(0)}(n,n)a^{(0)}(n,n-1)+a^{(0)}(n,n-1)$$

$$\times a^{(0)}(n-1,n-1)+\frac{1}{2}[a^{(0)}(n,n+1)a^{(0)}(n+1,n-1)$$

$$+a^{(0)}(n,n-2)a^{(0)}(n-2,n-1)]\}$$

$$=-\frac{5}{24}m\lambda\beta^3 n\sqrt{n}. \quad (B1)$$

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

$$-\frac{1}{8}\lambda m\{\omega^{(0)}(n,n+1)\omega^{(0)}(n+1,n-1)a^{(0)}(n,n+1)$$

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

$$\times a^{(0)}(n,n-2)a^{(0)}(n-2,n-1)\}=\frac{1}{12}m\lambda\beta^3 n\sqrt{n}. \quad (B2)$$

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

$$\frac{1}{24}m\lambda\{a^{(0)}(n,n-1)a^{(0)}(n-1,n)a^{(0)}(n,n-1)$$

$$+a^{(0)}(n,n-1)a^{(0)}(n-1,n-2)a^{(0)}(n-2,n-1)$$

$$+a^{(0)}(n,n+1)a^{(0)}(n+1,n)a^{(0)}(n,n-1)\}$$

$$=\frac{1}{8}m\lambda\beta^3 n\sqrt{n}. \quad (B3)$$

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

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

which is canceled by the corresponding term from $\frac{1}{2}m\dot{\hat{x}}^2$. 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 $\frac{1}{2}m\omega_0^2\hat{x}^2$:

$$\frac{1}{8}m\omega_0^2\lambda\{a^{(0)}(n,n-1)a^{(0)}(n-1,n-3)$$

$$+a^{(0)}(n,n-2)a^{(0)}(n-2,n-3)\}$$

$$=\frac{1}{24}m\lambda\beta^3\sqrt{n(n-1)(n-2)}. \quad (B5)$$

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

$$-\frac{1}{8}m\lambda\{\omega^{(0)}(n,n-1)a^{(0)}(n,n-1)\omega^{(0)}(n-1,n-3)$$

$$\times a^{(0)}(n-1,n-3)+\omega^{(0)}(n,n-2)$$

$$\times a^{(0)}(n,n-2)\omega^{(0)}(n-2,n-3)a^{(0)}(n-2,n-3)\}$$

$$=-\frac{1}{12}\lambda m\beta^3\sqrt{n(n-1)(n-2)}. \quad (B6)$$

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

$$\tfrac{1}{24} m\lambda a^{(0)}(n,n-1) a^{(0)}(n-1,n-2) a^{(0)}(n-2,n-3)$$

$$= \tfrac{1}{24} \lambda m \beta^3 \sqrt{n(n-1)(n-2)}. \tag{B7}$$

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

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

[2] This 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.

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

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

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

[7] S. 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.

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

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

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

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

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

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

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

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

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

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

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

[19] Of 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.

[20] Reference 7, p. 53.

[21] Reference 2, p. 262.

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

[23] We use ω rather than Heisenberg's ν.

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

[25] The 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.

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

[27] The 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 $\omega(n-|\alpha|, n)$.

[28] Conventional 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.

[29] Reference 2, p. 264.

[30] Reference 2, p. 265.

[31] Reference 2, p. 266.

[32] Reference 2 p. 267.

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

[34] Actually 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).

[35] W. Thomas, "Über die Zahl der Dispersionelektronen, die einem stationären Zustande zugeordnet sind (Vorläufige Mitteilung)," Naturwissenschaften **13**, 627 (1925).

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

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

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

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

[40] Reference 9, p. 202.

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

[42] For 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.

[43] See Ref. 3, p. 37.

[44] Reference 2, p. 268.

[45] For 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.

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

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

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

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

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

[51] MacKinnon (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).

[52] In 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.

[53] Heisenberg omitted the superscripts.

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

[55] Reference 2, p. 272.

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

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

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

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

[60] See Ref. 4, p. 305.

[61] Reference 57, p. 136.

[62] Reference 2, pp. 272–3.

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

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

The 1925 Born and Jordan paper "On quantum mechanics"

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The 1925 paper "On quantum mechanics" by M. Born and P. Jordan, and the sequel "On quantum mechanics II" by M. Born, W. Heisenberg, and P. Jordan, developed Heisenberg's pioneering theory into the first complete formulation of quantum mechanics. The Born and Jordan paper is the subject of the present article. This paper introduced matrices to physicists. We discuss the original postulates of quantum mechanics, present the two-part discovery of the law of commutation, and clarify the origin of Heisenberg's equation. We show how the 1925 proof of energy conservation and Bohr's frequency condition served as the gold standard with which to measure the validity of the new quantum mechanics. © *2009 American Association of Physics Teachers.*
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I. INTRODUCTION

The name "quantum mechanics" was coined by Max Born.[1] For Born and others, quantum mechanics denoted a canonical theory of atomic and electronic motion of the same level of generality and consistency as classical mechanics. The transition from classical mechanics to a true quantum mechanics remained an elusive goal prior to 1925.

Heisenberg made the breakthrough in his historic 1925 paper, "Quantum-theoretical reinterpretation of kinematic and mechanical relations."[2] Heisenberg's bold idea was to retain the classical equations of Newton but to replace the classical position coordinate with a "quantum-theoretical quantity." The new position quantity contains information about the measurable line spectrum of an atom rather than the unobservable orbit of the electron. Born realized that Heisenberg's kinematical rule for multiplying position quantities was equivalent to the mathematical rule for multiplying matrices. The next step was to formalize Heisenberg's theory using the language of matrices.

The first comprehensive exposition on quantum mechanics in matrix form was written by Born and Jordan,[4] and the sequel was written by Born, Heisenberg, and Jordan.[5] Dirac independently discovered the general equations of quantum mechanics without using matrix theory.[6] These papers developed a Hamiltonian mechanics of the atom in a completely new quantum (noncommutative) format. These papers ushered in a new era in theoretical physics where Hermitian matrices, commutators, and eigenvalue problems became the mathematical trademark of the atomic world. We discuss the first paper "On quantum mechanics."[4]

This formulation of quantum mechanics, now referred to as matrix mechanics,[7] marked one of the most intense periods of discovery in physics. The ideas and formalism behind the original matrix mechanics are absent in most textbooks. Recent articles discuss the correspondence between classical harmonics and quantum jumps,[8] the calculational details of Heisenberg's paper,[9] and the role of Born in the creation of quantum theory.[10] References 11–19 represent a sampling of the many sources on the development of quantum mechanics.

Given Born and Jordan's pivotal role in the discovery of quantum mechanics, it is natural to wonder why there are no equations named after them,[20] and why they did not share the Nobel Prize with others.[21] In 1933 Heisenberg wrote Born saying "The fact that I am to receive the Nobel Prize alone, for work done in Göttingen in collaboration—you, Jordan, and I, this fact depresses me and I hardly know what to write to you. I am, of course, glad that our common efforts are now appreciated, and I enjoy the recollection of the beautiful time of collaboration. I also believe that all good physicists know how great was your and Jordan's contribution to the structure of quantum mechanics—and this remains unchanged by a wrong decision from outside. Yet I myself can do nothing but thank you again for all the fine collaboration and feel a little ashamed."[23]

Engraved on Max Born's tombstone is a one-line epitaph: $pq-qp=h/2\pi i$. Born composed this elegant equation in early July 1925 and called it "die verschärfte Quantenbedingung"[4]—the sharpened quantum condition. This equation is now known as the law of commutation and is the hallmark of quantum algebra.

In the contemporary approach to teaching quantum mechanics, matrix mechanics is usually introduced after a thorough discussion of wave mechanics. The Heisenberg picture is viewed as a unitary transformation of the Schrödinger picture.[24] How was matrix mechanics formulated in 1925 when the Schrödinger picture was nowhere in sight? The Born and Jordan paper[4] represents matrix mechanics in its purest form.

II. BACKGROUND TO "ON QUANTUM MECHANICS"

Heisenberg's program, as indicated by the title of his paper,[2] consisted of constructing quantum-theoretical relations by reinterpreting the classical relations. To appreciate what Born and Jordan did with Heisenberg's reinterpretations, we discuss in the Appendix four key relations from Heisenberg's paper.[2] Heisenberg wrote the classical and quantum versions of each relation in parallel—as formula couplets. Heisenberg has been likened to an "expert decoder who reads a cryptogram."[25] The correspondence principle[8,26] acted as a "code book" for translating a classical relation into its quantum counterpart. Unlike his predecessors who used the correspondence principle to produce specific relations, Heisenberg produced an entirely new theory—complete with a new representation of position and a new rule of multiplication, together with an equation of motion and a quantum condition whose solution determined the atomic observables (energies, frequencies, and transition amplitudes).

Matrices are not explicitly mentioned in Heisenberg's paper. He did not arrange his quantum-theoretical quantities into a table or array. In looking back on his discovery, Heisenberg wrote, "At that time I must confess I did not know what a matrix was and did not know the rules of matrix multiplication."[18] In the last sentence of his paper he wrote "whether this method after all represents far too rough an approach to the physical program 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."[27]

Born took up Heisenberg's challenge to pursue "a more intensive mathematical investigation." At the time Heisenberg wrote his paper, he was Born's assistant at the University of Göttingen. Born recalls the moment of inspiration when he realized that position and momentum were matrices:[28]

> After having sent Heisenberg's paper to the Zeitschrift für Physik for publication, I began to ponder about his symbolic multiplication, and was soon so involved in it…For I felt there was something fundamental behind it…And one morning, about 10 July 1925, I suddenly saw the light: Heisenberg's symbolic multiplication was nothing but the matrix calculus, well known to me since my student days from the lectures of Rosanes in Breslau.

> I found this by just simplifying the notation a little: instead of $q(n, n+\tau)$, where n is the quantum number of one state and τ the integer indicating the transition, I wrote $q(n, m)$, and rewriting Heisenberg's form of Bohr's quantum condition, I recognized at once its formal significance. It meant that the two matrix products **pq** and **qp** are not identical. I was familiar with the fact that matrix multiplication is not commutative; therefore I was not too much puzzled by this result. Closer inspection showed that Heisenberg's formula gave only the value of the diagonal elements $(m=n)$ of the matrix **pq** − **qp**; it said they were all equal and had the value $h/2\pi i$ where h is Planck's constant and $i = \sqrt{-1}$. But what were the other elements $(m \neq n)$?

> Here my own constructive work began. Repeating Heisenberg's calculation in matrix notation, I soon convinced myself that the only reasonable value of the nondiagonal elements should be zero, and I wrote the strange equation

$$\mathbf{pq} - \mathbf{qp} = \frac{h}{2\pi i}\mathbf{1}, \qquad (1)$$

> where **1** is the unit matrix. But this was only a guess, and all my attempts to prove it failed.

On 19 July 1925, Born invited his former assistant Wolf-gang Pauli to collaborate on the matrix program. Pauli declined the invitation.[29] The next day, Born asked his student Pascual Jordan to assist him. Jordan accepted the invitation and in a few days proved Born's conjecture that all nondiagonal elements of **pq** − **qp** must vanish. The rest of the new quantum mechanics rapidly solidified. The Born and Jordan paper was received by the Zeitschrift für Physik on 27 September 1925, two months after Heisenberg's paper was received by the same journal. All the essentials of matrix mechanics as we know the subject today fill the pages of this paper.

In the abstract Born and Jordan wrote "The recently published theoretical approach of Heisenberg is here developed into a systematic theory of quantum mechanics (in the first place for systems having one degree of freedom) with the aid of mathematical matrix methods."[30] In the introduction they go on to write "The physical reasoning which led Heisenberg to this development has been so clearly described by him that any supplementary remarks appear superfluous. But, as he himself indicates, in its formal, mathematical aspects his approach is but in its initial stages. His hypotheses have been applied only to simple examples without being fully carried through to a generalized theory. Having been in an advantageous position to familiarize ourselves with his ideas throughout their formative stages, we now strive (since his investigations have been concluded) to clarify the mathematically formal content of his approach and present some of our results here. These indicate that it is in fact possible, starting with the basic premises given by Heisenberg, to build up a closed mathematical theory of quantum mechanics which displays strikingly close analogies with classical mechanics, but at the same time preserves the characteristic features of quantum phenomena."[31]

The reader is introduced to the notion of a matrix in the third paragraph of the introduction: "The mathematical basis of Heisenberg's treatment is the *law of multiplication* of quantum-theoretical quantities, which he derived from an ingenious consideration of correspondence arguments. The development of his formalism, which we give here, is based upon the fact that this rule of multiplication is none other than the well-known mathematical rule of *matrix multiplication*. The infinite square array which appears at the start of the next section, termed a *matrix*, is a representation of a physical quantity which is given in classical theory as a function of time. The mathematical method of treatment inherent in the new quantum mechanics is thereby characterized by the employment of *matrix analysis* in place of the usual number analysis."

The Born-Jordan paper[4] is divided into four chapters. Chapter 1 on "Matrix calculation" introduces the mathematics (algebra and calculus) of matrices to physicists. Chapter 2 on "Dynamics" establishes the fundamental postulates of quantum mechanics, such as the law of commutation, and derives the important theorems, such as the conservation of energy. Chapter 3 on "Investigation of the anharmonic oscillator" contains the first rigorous (correspondence free) calculation of the energy spectrum of a quantum-mechanical harmonic oscillator. Chapter 4 on "Remarks on electrodynamics" contains a procedure—the first of its kind—to quantize the electromagnetic field. We focus on the material in Chap. 2 because it contains the essential physics of matrix mechanics.

III. THE ORIGINAL POSTULATES OF QUANTUM MECHANICS

Current presentations of quantum mechanics frequently are based on a set of postulates.[32] The Born–Jordan postulates of quantum mechanics were crafted before wave mechanics was formulated and thus are quite different than the Schrödinger-based postulates in current textbooks. The original postulates come as close as possible to the classical-mechanical laws while maintaining complete quantum-mechanical integrity.

Section III, "The basic laws," in Chap. 2 of the Born–Jordan paper is five pages long and contains approximately thirty equations. We have imposed a contemporary postulatory approach on this section by identifying five fundamental passages from the text. We call these five fundamental ideas "the postulates." We have preserved the original phrasing, notation, and logic of Born and Jordan. The labeling and the naming of the postulates is ours.

Postulate 1. Position and Momentum. Born and Jordan introduce the position and momentum matrices by writing that[33]

> The dynamical system is to be described by the spatial coordinate **q** and the momentum **p**, these being represented by the matrices
>
> $$(\mathbf{q} = q(nm)e^{2\pi i \nu(nm)t}),$$
>
> $$(\mathbf{p} = p(nm)e^{2\pi i \nu(nm)t}). \qquad (2)$$
>
> Here the $\nu(nm)$ denote the quantum-theoretical frequencies associated with the transitions between states described by the *quantum numbers n and m*. The matrices (2) are to be Hermitian, e.g., on transposition of the matrices, each element is to go over into its complex conjugate value, a condition which should apply for all real t. We thus have
>
> $$q(nm)q(mn) = |q(nm)|^2 \qquad (3)$$
>
> and
>
> $$\nu(nm) = -\nu(mn). \qquad (4)$$
>
> If q is a *Cartesian* coordinate, then the expression (3) is a measure of the *probabilities* of the transitions $n \rightleftarrows m$.

The preceding passage placed Hermitian matrices into the physics limelight. Prior to the Born–Jordan paper, matrices were rarely seen in physics.[34] Hermitian matrices were even stranger. Physicists were reluctant to accept such an abstract mathematical entity as a description of physical reality.

For Born and Jordan, **q** and **p** do not specify the position and momentum of an electron in an atom. Heisenberg stressed that quantum theory should focus only on the observable properties, namely the frequency and intensity of the atomic radiation and not the position and period of the electron. The quantities **q** and **p** represent position and momentum in the sense that **q** and **p** satisfy matrix equations of motion that are identical in form to those satisfied by the position and momentum of classical mechanics. In the Bohr atom the electron undergoes periodic motion in a well defined orbit around the nucleus with a certain classical frequency. In the Heisenberg–Born–Jordan atom there is no longer an orbit, but there is some sort of periodic "quantum motion" of the electron characterized by the set of frequencies $\nu(nm)$ and amplitudes $q(nm)$. Physicists believed that something inside the atom must vibrate with the right frequencies even though they could not visualize what the quantum oscillations looked like. The mechanical properties $(\mathbf{q}, \mathbf{p})$ of the quantum motion contain complete information on the spectral properties (frequency, intensity) of the emitted radiation.

The diagonal elements of a matrix correspond to the states, and the off-diagonal elements correspond to the transitions. An important property of all dynamical matrices is that the diagonal elements are independent of time. The Hermitian rule in Eq. (4) implies the relation $\nu(nn) = 0$. Thus the time factor of the nth diagonal term in any matrix is $e^{2\pi i \nu(nn)t} = 1$. As we shall see, the time-independent entries in a diagonal matrix are related to the constant values of a conserved quantity.

In their purely mathematical introduction to matrices (Chap. 1), Born and Jordan use the following symbols to denote a matrix

$$\mathbf{a} = (a(nm)) = \begin{pmatrix} a(00) & a(01) & a(02) & \dots \\ a(10) & a(11) & a(12) & \\ a(20) & a(21) & a(22) & \\ \vdots & & & \ddots \end{pmatrix}. \qquad (5)$$

The bracketed symbol $(a(nm))$, which displays inner elements $a(nm)$ contained within outer brackets ( ), is the shorthand notation for the array in Eq. (5). By writing the matrix elements as $a(nm)$, rather than a_{nm}, Born and Jordan made direct contact with Heisenberg's quantum-theoretical quantities $a(n, n-\alpha)$ (see the Appendix). They wrote[35] "Matrix multiplication is defined by the rule 'rows times columns,' familiar from the ordinary theory of determinants:

$$\mathbf{a} = \mathbf{bc} \text{ means } a(nm) = \sum_{k=0}^{\infty} b(nk)c(km). \text{"} \qquad (6)$$

This multiplication rule was first given (for finite square matrices) by Arthur Cayley.[36] Little did Cayley know in 1855 that his mathematical "row times column" expression $b(nk)c(km)$ would describe the physical process of an electron making the transition $n \rightarrow k \rightarrow m$ in an atom.

Born and Jordan wrote in Postulate 1 that the quantity $|q(nm)|^2$ provides "a measure of the *probabilities* of the transitions $n \rightleftarrows m$." They justify this profound claim in the last chapter.[37] Born and Jordan's one-line claim about transition probabilities is the only statistical statement in their postulates. Physics would have to wait several months before Schrödinger's wave function $\Psi(x)$ and Born's probability function $|\Psi(x)|^2$ entered the scene. Born discovered the connection between $|\Psi(x)|^2$ and position probability, and was also the first physicist (with Jordan) to formalize the connection between $|q(nm)|^2$ and the transition probability via a "quantum electrodynamic" argument.[38] As a pioneer statistical interpreter of quantum mechanics, it is interesting to speculate that Born might have discovered how to form a

linear superposition of the periodic matrix elements $q(nm)e^{2\pi i\nu(nm)t}$ in order to obtain another statistical object, namely the expectation value $\langle \mathbf{q} \rangle$. Early on, Born, Heisenberg, and Jordan did superimpose matrix elements,[47] but did not supply the statistical interpretation.

Postulate 2. Frequency Combination Principle. After defining $\mathbf{q}$ and $\mathbf{p}$, Born and Jordan wrote[39] "Further, we shall require that

$$\nu(jk) + \nu(kl) + \nu(lj) = 0 . "\tag{7}$$

The frequency sum rule in Eq. (7) is the fundamental constraint on the quantum-theoretical frequencies. This rule is based on the Ritz combination principle, which explains the relations of the spectral lines of atomic spectroscopy.[40] Equation (7) is the quantum analogue of the "Fourier combination principle", $\nu(k-j) + \nu(l-k) + \nu(j-l) = 0$, where $\nu(\alpha) = \alpha\nu(1)$ is the frequency of the αth harmonic component of a Fourier series. The frequency spectrum of classical periodic motion obeys this Fourier sum rule. The equal Fourier spacing of classical lines is replaced by the irregular Ritzian spacing of quantal lines. In the correspondence limit of large quantum numbers and small quantum jumps the atomic spectrum of Ritz reduces to the harmonic spectrum of Fourier.[8,26] Because the Ritz rule was considered an exact law of atomic spectroscopy, and because Fourier series played a vital role in Heisenberg's analysis, it made sense for Born and Jordan to posit the frequency rule in Eq. (7) as a basic law.

One might be tempted to regard Eq. (7) as equivalent to the Bohr frequency condition, $E(n) - E(m) = h\nu(nm)$, where $E(n)$ is the energy of the stationary state n. For Born and Jordan, Eq. (7) says nothing about energy. They note that Eqs. (4) and (7) imply that there exists spectral terms W_n such that

$$h\nu(nm) = W_n - W_m.\tag{8}$$

At this postulatory stage, the term W_n of the spectrum is unrelated to the energy $E(n)$ of the state. Heisenberg emphasized this distinction between "term" and "energy" in a letter to Pauli summarizing the Born–Jordan theory.[41] Born and Jordan adopt Eq. (7) as a postulate–one based solely on the observable spectral quantities $\nu(nm)$ without reference to any mechanical quantities $E(n)$. The Bohr frequency condition is not something they assume *a priori*, it is something that must be rigorously proved.

The Ritz rule insures that the nm element of any dynamical matrix (any function of $\mathbf{p}$ and $\mathbf{q}$) oscillates with the same frequency $\nu(nm)$ as the nm element of $\mathbf{p}$ and $\mathbf{q}$. For example, if the $3 \rightarrow 2$ elements of $\mathbf{p}$ and $\mathbf{q}$ oscillate at 500 MHz, then the $3 \rightarrow 2$ elements of $\mathbf{p}^2$, $\mathbf{q}^2$, $\mathbf{pq}$, $\mathbf{q}^3$, $\mathbf{p}^2 + \mathbf{q}^2$, etc. each oscillate at 500 MHz. In all calculations involving the canonical matrices $\mathbf{p}$ and $\mathbf{q}$, no new frequencies are generated. A consistent quantum theory must preserve the frequency spectrum of a particular atom because the spectrum is the spectroscopic signature of the atom. The calculations must not change the identity of the atom. Based on the rules for manipulating matrices and combining frequencies, Born and Jordan wrote that "it follows that a function $\mathbf{g}(\mathbf{pq})$ invariably takes on the form

$$\mathbf{g} = (g(nm)e^{2\pi i\nu(nm)t})\tag{9}$$

and the matrix $(g(nm))$ therein results from identically same process applied to the matrices $(q(nm))$, $(p(nm))$ as

was employed to find $\mathbf{g}$ from $\mathbf{q}$, $\mathbf{p}$."[42] Because $e^{2\pi i\nu(nm)t}$ is the universal time factor common to all dynamical matrices, they note that it can be dropped from Eq. (2) in favor of the shorter notation $\mathbf{q} = (q(nm))$ and $\mathbf{p} = (p(nm))$.

Why does the Ritz rule insure that the time factors of $\mathbf{g}(\mathbf{pq})$ are identical to the time factors of $\mathbf{p}$ and $\mathbf{q}$? Consider the potential energy function $\mathbf{q}^2$. The nm element of $\mathbf{q}^2$, which we denote by $\mathbf{q}^2(nm)$, is obtained from the elements of $\mathbf{q}$ via the multiplication rule

$$\mathbf{q}^2(nm) = \sum_k q(nk)e^{2\pi i\nu(nk)t}q(km)e^{2\pi i\nu(km)t}.\tag{10}$$

Given the Ritz relation $\nu(nm) = \nu(nk) + \nu(km)$, which follows from Eqs. (4) and (7), Eq. (10) reduces to

$$\mathbf{q}^2(nm) = \left[\sum_k q(nk)q(km)\right]e^{2\pi i\nu(nm)t}.\tag{11}$$

It follows that the nm time factor of $\mathbf{q}^2$ is the same as the nm time factor of $\mathbf{q}$.

We see that the theoretical rule for multiplying mechanical amplitudes, $a(nm) = \sum_k b(nk)c(km)$, is intimately related to the experimental rule for adding spectral frequencies, $\nu(nm) = \nu(nk) + \nu(km)$. The Ritz rule occupied a prominent place in Heisenberg's discovery of the multiplication rule (see the Appendix). Whenever a contemporary physicist calculates the total amplitude of the quantum jump $n \rightarrow k \rightarrow m$, the steps involved can be traced back to the frequency combination principle of Ritz.

Postulate 3. The Equation of Motion. Born and Jordan introduce the law of quantum dynamics by writing[43]

In the case of a Hamilton function having the form

$$\mathbf{H} = \frac{1}{2m}\mathbf{p}^2 + \mathbf{U}(\mathbf{q}),\tag{12}$$

we shall assume, as did Heisenberg, that the equations of motion have just the same form as in the classical theory, so that we can write:

$$\dot{\mathbf{q}} = \frac{\partial \mathbf{H}}{\partial \mathbf{p}} = \frac{1}{m}\mathbf{p},\tag{13a}$$

$$\dot{\mathbf{p}} = -\frac{\partial \mathbf{H}}{\partial \mathbf{q}} = -\frac{\partial \mathbf{U}}{\partial \mathbf{q}}.\tag{13b}$$

This Hamiltonian formulation of quantum dynamics generalized Heisenberg's Newtonian approach.[44] The assumption by Heisenberg and Born and Jordan that quantum dynamics looks the same as classical dynamics was a bold and deep assumption. For them, the problem with classical mechanics was not the dynamics (the form of the equations of motion), but rather the kinematics (the meaning of position and momentum).

Postulate 4. Energy Spectrum. Born and Jordan reveal the connection between the allowed energies of a conservative system and the numbers in the Hamiltonian matrix:

"The diagonal elements $H(nn)$ of $\mathbf{H}$ are interpreted, according to Heisenberg, as the *energies of the various states of the system.*"[45]

This statement introduced a radical new idea into mainstream physics: calculating an energy spectrum reduces to finding the components of a diagonal matrix.[46] Although Born and Jordan did not mention the word eigenvalue in Ref. 4, Born, Heisenberg, and Jordan would soon formalize the idea of calculating an energy spectrum by solving an eigenvalue problem.[5] The ad hoc rules for calculating a quantized energy in the old quantum theory were replaced by a systematic mathematical program.

Born and Jordan considered exclusively conservative systems for which $\mathbf{H}$ does not depend explicitly on time. The connection between conserved quantities and diagonal matrices will be discussed later. For now, recall that the diagonal elements of any matrix are independent of time. For the special case where all the non-diagonal elements of a dynamical matrix $\mathbf{g}(\mathbf{pq})$ vanish, the quantity $\mathbf{g}$ is a constant of the motion. A postulate must be introduced to specify the physical meaning of the constant elements in $\mathbf{g}$.

In the old quantum theory it was difficult to explain why the energy was quantized. The discontinuity in energy had to be postulated or artificially imposed. Matrices are naturally quantized. The quantization of energy is built into the discrete row-column structure of the matrix array. In the old theory Bohr's concept of a stationary state of energy E_n was a central concept. Physicists grappled with the questions: Where does E_n fit into the theory? How is E_n calculated? Bohr's concept of the energy of the stationary state finally found a rigorous place in the new matrix scheme.[47]

Postulate 5. The Quantum Condition. Born and Jordan state that the elements of $\mathbf{p}$ and $\mathbf{q}$ for any quantum mechanical system must satisfy the "quantum condition":

$$\sum_k (p(nk)q(kn) - q(nk)p(kn)) = \frac{h}{2\pi i}. \tag{14}$$

Given the significance of Eq. (14) in the development of quantum mechanics, we quote Born and Jordan's "derivation" of this equation:

The equation

$$J = \oint p dq = \int_0^{1/\nu} p\dot{q}dt \tag{15}$$

of "classical" quantum theory can, on introducing the Fourier expansions of p and q,

$$p = \sum_{\tau=-\infty}^{\infty} p_\tau e^{2\pi i \nu \tau t},$$

$$q = \sum_{\tau=-\infty}^{\infty} q_\tau e^{2\pi i \nu \tau t}, \tag{16}$$

be transformed into

$$1 = 2\pi i \sum_{\tau=-\infty}^{\infty} \tau \frac{\partial}{\partial J}(q_\tau p_{-\tau}). \tag{17}$$

The following expressions should correspond:

$$\sum_{\tau=-\infty}^{\infty} \tau \frac{\partial}{\partial J}(q_\tau p_{-\tau}) \tag{18}$$

with

$$\frac{1}{h} \sum_{\tau=-\infty}^{\infty} (q(n+\tau,n)p(n,n+\tau)$$

$$- q(n,n-\tau)p(n-\tau,n)), \tag{19}$$

where in the right-hand expression those $q(nm)$, $p(nm)$ which take on a negative index are to be set equal to zero. In this way we obtain the quantization condition corresponding to Eq. (17) as

$$\sum_k (p(nk)q(kn) - q(nk)p(kn)) = \frac{h}{2\pi i}. \tag{20}$$

This is a system of infinitely many equations, namely one for each value of n.[48]

Why did Born and Jordan take the derivative of the action integral in Eq. (15) to arrive at Eq. (17)? Heisenberg performed a similar maneuver (see the Appendix). One reason is to eliminate any explicit dependence on the integer variable n from the basic laws. Another reason is to generate a differential expression that can readily be translated via the correspondence principle into a difference expression containing only transition quantities. In effect, a state relation is converted into a change-in-state relation. In the old quantum theory the Bohr–Sommerfeld quantum condition, $\oint p dq = nh$, determined how all state quantities depend on n. Such an ad hoc quantization algorithm has no proper place in a rigorous quantum theory, where n should not appear explicitly in any of the fundamental laws. The way in which $q(nm)$, $p(nm)$, $\nu(nm)$ depend on (nm) should not be artificially imposed, but should be naturally determined by fundamental relations involving only the canonical variables $\mathbf{q}$ and $\mathbf{p}$, without any explicit dependence on the state labels n and m. Equation (20) is one such fundamental relation.

In 1924 Born introduced the technique of replacing differentials by differences to make the "formal passage from classical mechanics to a 'quantum mechanics'."[49] This correspondence rule played an important role in allowing Born and others to develop the equations of quantum mechanics.[50] To motivate Born's rule note that the fundamental orbital frequency of a classical periodic system is equal to dE/dJ (E is energy and $J = \oint p dq$ is an action),[51] whereas the spectral frequency of an atomic system is equal to $\Delta E/h$. Hence, the passage from a classical to a quantum frequency is made by replacing the derivative dE/dJ by the difference $\Delta E/h$.[52] Born conjectured that this correspondence is valid for any quantity Φ. He wrote "We are therefore as good as forced to adopt the rule that we have to replace a classically calculated quantity, whenever it is of the form $\tau \partial \Phi/\partial J$ by the linear average or difference quotient $[\Phi(n+\tau)-\Phi(n)]/h$."[53] The correspondence between Eqs. (18) and (19) follows from

Born's rule by letting Φ be $\Phi(n)=q(n,n-\tau)p(n-\tau,n)$, where $q(n,n-\tau)$ corresponds to q_τ and $p(n-\tau,n)$ corresponds to $p_{-\tau}$ or p_τ^*.

Born and Jordan remarked that Eq. (20) implies that **p** and **q** can never be finite matrices.[54] For the special case **p** $=m\dot{\mathbf{q}}$ they also noted that the general condition in Eq. (20) reduces to Heisenberg's form of the quantum condition (see the Appendix). Heisenberg did not realize that his quantization rule was a relation between **pq** and **qp**.[55]

Planck's constant h enters into the theory via the quantum condition in Eq. (20). The quantum condition expresses the following deep law of nature: *All the diagonal components of* **pq**−**qp** *must equal the universal constant* $h/2\pi i$.

What about the nondiagonal components of **pq**−**qp**? Born claimed that they were all equal to zero. Jordan proved Born's claim. It is important to emphasize that Postulate 5 says nothing about the nondiagonal elements. Born and Jordan were careful to distinguish the postulated statements (laws of nature) from the derivable results (consequences of the postulates). Born's development of the diagonal part of **pq**−**qp** and Jordan's derivation of the nondiagonal part constitute the two-part discovery of the law of commutation.

IV. THE LAW OF COMMUTATION

Born and Jordan write the following equation in Sec. IV of "On quantum mechanics":

$$\mathbf{pq}-\mathbf{qp}=\frac{h}{2\pi i}\mathbf{1}. \tag{21}$$

They call Eq. (21) the "sharpened quantum condition" because it sharpened the condition in Eq. (20), which only fixes the diagonal elements, to one which fixes all the elements. In a letter to Pauli, Heisenberg referred to Eq. (21) as a "fundamental law of this mechanics" and as "Born's very clever idea."[56] Indeed, the commutation law in Eq. (21) is one of the most fundamental relations in quantum mechanics. This equation introduces Planck's constant and the imaginary number i into the theory in the most basic way possible. It is the golden rule of quantum algebra and makes quantum calculations unique. The way in which all dynamical properties of a system depend on h can be traced back to the simple way in which **pq**−**qp** depend on h. In short, the commutation law in Eq. (21) stores information on the discontinuity, the non-commutativity, the uncertainty, and the complexity of the quantum world.

In their paper Born and Jordan proved that the off-diagonal elements of **pq**−**qp** are equal to zero by first establishing a "diagonality theorem," which they state as follows: "If $\nu(nm)\neq0$ when $n\neq m$, a condition which we wish to assume, then the formula $\dot{\mathbf{g}}=0$ denotes that **g** is a diagonal matrix with $g(nm)=\delta_{nm}g(nn)$."[57] This theorem establishes the connection between the structural (diagonality) and the temporal (constancy) properties of a dynamical matrix. It provided physicists with a whole new way to look at conservation principles: *In quantum mechanics, conserved quantities are represented by diagonal matrices.*[58]

Born and Jordan proved the diagonality theorem as follows. Because all dynamical matrices **g**(**pq**) have the form in Eq. (9), the time derivative of **g** is

$$\dot{\mathbf{g}}=2\pi i(\nu(nm)g(nm)e^{2\pi i\nu(nm)t}). \tag{22}$$

If $\dot{\mathbf{g}}=0$, then Eq. (22) implies the relation $\nu(nm)g(nm)=0$ for all (nm). This relation is always true for the diagonal elements because $\nu(nn)$ is always equal to zero. For the off-diagonal elements, the relation $\nu(nm)g(nm)=0$ implies that $g(nm)$ must equal zero, because it is assumed that $\nu(nm)\neq0$ for $n\neq m$. Thus, **g** is a diagonal matrix.

Hence, to show that **pq**−**qp** is a diagonal matrix, Born and Jordan showed that the time derivative of **pq**−**qp** is equal to zero. They introduced the matrix $\mathbf{d}\equiv\mathbf{pq}-\mathbf{qp}$ and expressed the time derivative of **d** as

$$\dot{\mathbf{d}}=\dot{\mathbf{p}}\mathbf{q}+\mathbf{p}\dot{\mathbf{q}}-\dot{\mathbf{q}}\mathbf{p}-\mathbf{q}\dot{\mathbf{p}}. \tag{23}$$

They used the canonical equations of motion in Eq. (13) to write Eq. (23) as

$$\dot{\mathbf{d}}=\mathbf{q}\frac{\partial\mathbf{H}}{\partial\mathbf{q}}-\frac{\partial\mathbf{H}}{\partial\mathbf{q}}\mathbf{q}+\mathbf{p}\frac{\partial\mathbf{H}}{\partial\mathbf{p}}-\frac{\partial\mathbf{H}}{\partial\mathbf{p}}\mathbf{p}. \tag{24}$$

They next demonstrated that the combination of derivatives in Eq. (24) leads to a vanishing result[59] and say that "it follows that $\dot{\mathbf{d}}=0$ and **d** is a diagonal matrix. The diagonal elements of **d** are, however, specified by the quantum condition (20). Summarizing, we obtain the equation

$$\mathbf{pq}-\mathbf{qp}=\frac{h}{2\pi i}\mathbf{1}, \tag{25}$$

on introducing the unit matrix **1**. We call Eq. (25) the 'sharpened quantum condition' and base all further conclusions on it."[60] Fundamental results that propagate from Eq. (25) include the equation of motion, $\dot{\mathbf{g}}=(2\pi i/h)(\mathbf{Hg}-\mathbf{gH})$ (see Sec. V), the Heisenberg uncertainty principle, $\Delta p\Delta q\geq h/4\pi$, and the Schrödinger operator, $p=(h/2\pi i)d/dq$.

It is important to emphasize the two distinct origins of $\mathbf{pq}-\mathbf{qp}=(h/2\pi i)\mathbf{1}$. The diagonal part, $(\mathbf{pq}-\mathbf{qp})_{\text{diagonal}}=h/2\pi i$ is a *law*—an exact decoding of the approximate law $\oint p\,dq=nh$. The nondiagonal part, $(\mathbf{pq}-\mathbf{qp})_{\text{nondiagonal}}=0$, is a *theorem*—a logical consequence of the equations of motion. From a practical point of view Eq. (25) represents vital information on the line spectrum of an atom by defining a system of algebraic equations that place strong constraints on the magnitudes of $q(nm)$, $p(nm)$, and $\nu(nm)$.

V. THE EQUATION OF MOTION

Born and Jordan proved that the equation of motion describing the time evolution of any dynamical quantity $\mathbf{g}(\mathbf{pq})$ is

$$\dot{\mathbf{g}}=\frac{2\pi i}{h}(\mathbf{Hg}-\mathbf{gH}). \tag{26}$$

Equation (26) is now often referred to as the Heisenberg equation.[61] In Ref. 2 the only equation of motion is Newton's second law, which Heisenberg wrote as $\ddot{x}+f(x)=0$ (see the Appendix).

The "commutator" of mechanical quantities is a recurring theme in the Born–Jordan theory. The quantity **pq**−**qp** lies at the core of their theory. Equation (26) reveals how the quantity **Hg**−**gH** is synonymous with the time evolution of **g**. Thanks to Born and Jordan, as well as Dirac who established the connection between commutators and classical Poisson

brackets,[6] the commutator is now an integral part of modern quantum theory. The change in focus from commuting variables to noncommuting variables represents a paradigm shift in quantum theory.

The original derivation of Eq. (26) is different from present-day derivations. In the usual textbook presentation Eq. (26) is derived from a unitary transformation of the states and operators in the Schrödinger picture.[24] In 1925, the Schrödinger picture did not exist. To derive Eq. (26) from their postulates Born and Jordan developed a new quantum-theoretical technology that is now referred to as "commutator algebra." They began the proof by stating the following generalizations of Eq. (25):

$$\mathbf{p}^n\mathbf{q} = \mathbf{q}\mathbf{p}^n + n\frac{h}{2\pi i}\mathbf{p}^{n-1}, \tag{27}$$

$$\mathbf{q}^n\mathbf{p} = \mathbf{p}\mathbf{q}^n - n\frac{h}{2\pi i}\mathbf{q}^{n-1}, \tag{28}$$

which can readily be derived by induction. They considered Hamiltonians of the form

$$\mathbf{H} = \mathbf{H}_1(\mathbf{p}) + \mathbf{H}_2(\mathbf{q}), \tag{29}$$

where $\mathbf{H}_1(\mathbf{p})$ and $\mathbf{H}_2(\mathbf{q})$ are represented by power series

$$\mathbf{H}_1 = \sum_s a_s\mathbf{p}^s, $$

$$\mathbf{H}_2 = \sum_s b_s\mathbf{q}^s. \tag{30}$$

After writing these expressions, they wrote[62] "Formulae (27) and (28) indicate that

$$\mathbf{H}\mathbf{q} - \mathbf{q}\mathbf{H} = \frac{h}{2\pi i}\frac{\partial \mathbf{H}}{\partial \mathbf{p}}, \tag{31}$$

$$\mathbf{H}\mathbf{p} - \mathbf{p}\mathbf{H} = -\frac{h}{2\pi i}\frac{\partial \mathbf{H}}{\partial \mathbf{q}}. \tag{32}$$

Comparison with the equations of motion (13) yields

$$\dot{\mathbf{q}} = \frac{2\pi i}{h}(\mathbf{H}\mathbf{q} - \mathbf{q}\mathbf{H}), \tag{33}$$

$$\dot{\mathbf{p}} = \frac{2\pi i}{h}(\mathbf{H}\mathbf{p} - \mathbf{p}\mathbf{H}). \tag{34}$$

Denoting the matrix $\mathbf{H}\mathbf{g} - \mathbf{g}\mathbf{H}$ by $\left|\begin{smallmatrix}\mathbf{H}\\\mathbf{g}\end{smallmatrix}\right|$ for brevity, one has

$$\left|\begin{matrix}\mathbf{H}\\\mathbf{ab}\end{matrix}\right| = \left|\begin{matrix}\mathbf{H}\\\mathbf{a}\end{matrix}\right|\mathbf{b} + \mathbf{a}\left|\begin{matrix}\mathbf{H}\\\mathbf{b}\end{matrix}\right|, \tag{35}$$

from which generally for $\mathbf{g} = \mathbf{g}(\mathbf{pq})$ one may conclude that

$$\dot{\mathbf{g}} = \frac{2\pi i}{h}\left|\begin{matrix}\mathbf{H}\\\mathbf{g}\end{matrix}\right| = \frac{2\pi i}{h}(\mathbf{H}\mathbf{g} - \mathbf{g}\mathbf{H}) . \text{ "} \tag{36}$$

The derivation of Eq. (36) clearly displays Born and Jordan's expertise in commutator algebra. The essential step to go from Eq. (27) to Eq. (31) is to note that Eq. (27) can be rewritten as a commutator-derivative relation, $\mathbf{p}^n\mathbf{q} - \mathbf{q}\mathbf{p}^n = (h/2\pi i)d\mathbf{p}^n/d\mathbf{p}$, which is equivalent to the nth term of the series representation of Eq. (31). The generalized commutation rules in Eqs. (27) and (28), and the relation between

commutators and derivatives in Eqs. (31) and (32) are now standard operator equations of contemporary quantum theory.

With the words, "Denoting the matrix $\mathbf{H}\mathbf{g} - \mathbf{g}\mathbf{H}$ by $\left|\begin{smallmatrix}\mathbf{H}\\\mathbf{g}\end{smallmatrix}\right|$," Born and Jordan formalized the notion of a commutator and introduced physicists to this important quantum-theoretical object. The appearance of Eq. (36) in Ref. 4 marks the first printed statement of the general equation of motion for a dynamical quantity in quantum mechanics.

VI. THE ENERGY THEOREMS

Heisenberg, Born, and Jordan considered the conservation of energy and the Bohr frequency condition as universal laws that should emerge as logical consequences of the fundamental postulates. Proving energy conservation and the frequency condition was the ultimate measure of the power of the postulates and the validity of the theory.[63] Born and Jordan began Sec. IV of Ref. 4 by writing "The content of the preceding paragraphs furnishes the basic rules of the new quantum mechanics in their entirety. All the other laws of quantum mechanics, whose general validity is to be verified, must be *derivable* from these basic tenets. As instances of such laws to be proved, the law of energy conservation and the Bohr frequency condition primarily enter into consideration."[64]

The energy theorems are stated as follows:[65]

$$\dot{\mathbf{H}} = 0 \quad \text{(energy conservation)}, \tag{37}$$

$$h\nu(nm) = H(nn) - H(mm) \quad \text{(frequency condition)}. \tag{38}$$

Equations (37) and (38) are remarkable statements on the temporal behavior of the system and the logical structure of the theory.[66] Equation (37) says that $\mathbf{H}$, which depends on the matrices $\mathbf{p}$ and $\mathbf{q}$ is always a constant of the motion even though $\mathbf{p} = \mathbf{p}(t)$ and $\mathbf{q} = \mathbf{q}(t)$ depend on time. In short, the t in $\mathbf{H}(\mathbf{p}(t), \mathbf{q}(t))$ must completely disappear. Equation (37) reveals the time independence of $\mathbf{H}$, and Eq. (38) specifies how $\mathbf{H}$ itself determines the time dependence of all other dynamical quantities.

Why should $\nu(nm)$, $H(nn)$, and $H(mm)$ be related? These quantities are completely different structural elements of different matrices. The parameter $\nu(nm)$ is a transition quantity that characterizes the off-diagonal, time-dependent part of $\mathbf{q}$ and $\mathbf{p}$. In contrast, $H(nn)$ is a state quantity that characterizes the diagonal, time-independent part of $\mathbf{H}(\mathbf{pq})$. It is a nontrivial claim to say that these mechanical elements are related.

It is important to distinguish between the Bohr meaning of $E_n - E_m = h\nu$ and the Born–Jordan meaning of $H(nn) - H(mm) = h\nu(nm)$. For Bohr, E_n denotes the mechanical energy of the electron and ν denotes the spectral frequency of the radiation. In the old quantum theory there exists ad hoc, semiclassical rules to calculate E_n. There did not exist any mechanical rules to calculate ν, independent of E_n and E_m. The relation between $E_n - E_m$ and ν was postulated. Born and Jordan did not postulate any connection between $H(nn)$, $H(mm)$, and $\nu(nm)$. The basic mechanical laws (law of motion and law of commutation) allow them to calculate the frequencies $\nu(nm)$ which paramaterize $\mathbf{q}$ and the energies $H(nn)$ stored in $\mathbf{H}$. The theorem in Eq. (38) states that the

calculated values of the mechanical parameters $H(nn)$, $H(mm)$, and $\nu(nm)$ will always satisfy the relation $H(nn) - H(mm) = h\nu(nm)$.

The equation of motion (36) is the key to proving the energy theorems. Born and Jordan wrote "In particular, if in Eq. (36) we set $\mathbf{g} = \mathbf{H}$, we obtain

$$\dot{\mathbf{H}} = 0. \tag{39}$$

Now that we have verified the energy-conservation law and recognized the matrix $\mathbf{H}$ to be diagonal [by the diagonality theorem, $\dot{\mathbf{H}} = 0 \Rightarrow \mathbf{H}$ is diagonal], Eqs. (33) and (34) can be put into the form

$$h\nu(nm)q(nm) = (H(nn) - H(mm))q(nm), \tag{40}$$

$$h\nu(nm)p(nm) = (H(nn) - H(mm))p(nm), \tag{41}$$

from which the frequency condition follows."[67] Given the importance of this result, it is worthwhile to elaborate on the proof. Because the nm component of any matrix $\mathbf{g}$ is $g(nm)e^{2\pi i\nu(nm)t}$, the nm component of the matrix relation in Eq. (33) is

$$2\pi i\nu(nm)q(nm)e^{2\pi i\nu(nm)t}$$
$$= \frac{2\pi i}{h}\sum_k (H(nk)q(km)$$
$$- q(nk)H(km))e^{2\pi i[\nu(nk)+\nu(km)]t}. \tag{42}$$

Given the diagonality of $\mathbf{H}$, $H(nk) = H(nn)\delta_{nk}$ and $H(km) = H(mm)\delta_{km}$, and the Ritz rule, $\nu(nk) + \nu(km) = \nu(nm)$, Eq. (42) reduces to

$$\nu(nm) = \frac{1}{h}(H(nn) - H(mm)). \tag{43}$$

In this way Born and Jordan demonstrated how Bohr's frequency condition, $h\nu(nm) = H(nn) - H(mm)$, is simply a scalar component of the matrix equation, $h\dot{\mathbf{q}} = 2\pi i(\mathbf{Hq} - \mathbf{qH})$. In any presentation of quantum mechanics it is important to explain how and where Bohr's frequency condition logically fits into the formal structure.[68]

According to Postulate 4, the nth diagonal element $H(nn)$ of $\mathbf{H}$ is equal to the energy of the nth stationary state. Logically, this postulate is needed to interpret Eq. (38) as the original frequency condition conjectured by Bohr. Born and Jordan note that Eqs. (8) and (38) imply that the mechanical energy $H(nn)$ is related to the spectral term W_n as follows: $W_n = H(nn) + \text{constant}$.[69]

This mechanical proof of the Bohr frequency condition established an explicit connection between time evolution and energy. In the matrix scheme all mechanical quantities ($\mathbf{p}$, $\mathbf{q}$, and $\mathbf{g(pq)}$) evolve in time via the set of factors $e^{2\pi i\nu(nm)t}$, where $\nu(nm) = (H(nn) - H(mm))/h$. Thus, all $\mathbf{g}$-functions have the form[70]

$$\mathbf{g} = (g(nm)e^{2\pi i(H(nn)-H(mm))t/h}). \tag{44}$$

Equation (44) exhibits how the difference in energy between state n and state m is the "driving force" behind the time evolution (quantum oscillations) associated with the change of state $n \rightarrow m$.

In the introduction of their paper, Born and Jordan write "With the aid of [the equations of motion and the quantum

condition], one can prove the general validity of the *law of conservation of energy* and the *Bohr frequency relation* in the sense conjectured by Heisenberg: this proof could not be carried through in its entirety by him even for the simple examples which he considered."[71] Because $\mathbf{p}$ and $\mathbf{q}$ do not commute, the mechanism responsible for energy conservation in quantum mechanics is significantly different than the classical mechanism. Born and Jordan emphasize this difference by writing "Whereas in classical mechanics energy conservation ($\dot{H} = 0$) is directly apparent from the canonical equations, the same law of energy conservation in quantum mechanics, $\dot{H} = 0$ lies, as one can see, more deeply hidden beneath the surface. That its demonstrability from the assumed postulates is far from being trivial will be appreciated if, following more closely the classical method of proof, one sets out to prove $\mathbf{H}$ to be constant simply by evaluating $\dot{\mathbf{H}}$."[72]

We carry out Born and Jordan's suggestion "to prove $\mathbf{H}$ to be constant simply by evaluating $\dot{\mathbf{H}}$" for the special Hamiltonian

$$\mathbf{H} = \mathbf{p}^2 + \mathbf{q}^3. \tag{45}$$

In order to focus on the energy calculus of the $\mathbf{p}$ and $\mathbf{q}$ matrices, we have omitted the scalar coefficients in Eq. (45). If we write Eq. (45) as $\mathbf{H} = \mathbf{pp} + \mathbf{qqq}$, calculate $\dot{\mathbf{H}}$, and use the equations of motion $\dot{\mathbf{q}} = 2\mathbf{p}$, $\dot{\mathbf{p}} = -3\mathbf{q}^2$, we find[73]

$$\dot{\mathbf{H}} = \mathbf{q}(\mathbf{pq} - \mathbf{qp}) + (\mathbf{qp} - \mathbf{pq})\mathbf{q}. \tag{46}$$

Equation (46) reveals how the value of $\mathbf{pq} - \mathbf{qp}$ uniquely determines the value of $\dot{\mathbf{H}}$. The quantum condition, $\mathbf{pq} - \mathbf{qp} = (h/2\pi i)\mathbf{1}$, reduces Eq. (46) to $\dot{\mathbf{H}} = 0$. In classical mechanics the classical condition, $pq - qp = 0$, is taken for granted in proving energy conservation. In quantum mechanics the condition that specifies the nonzero value of $\mathbf{pq} - \mathbf{qp}$ plays a nontrivial role in establishing energy conservation. This nontriviality is what Born and Jordan meant when they wrote that energy conservation in quantum mechanics "lies more deeply hidden beneath the surface."

Proving the law of energy conservation and the Bohr frequency condition was the decisive test of the theory—the final validation of the new quantum mechanics. All of the pieces of the "quantum puzzle" now fit together. After proving the energy theorems, Born and Jordan wrote that "The fact that energy-conservation and frequency laws could be proved in so general a context would seem to us to furnish strong grounds to hope that this theory embraces truly deepseated physical laws."[74]

VII. CONCLUSION

To put the discovery of quantum mechanics in matrix form into perspective, we summarize the contributions of Heisenberg and Born–Jordan. Heisenberg's breakthrough consists of four quantum-theoretical reinterpretations (see the Appendix):

1. Replace the position coordinate $x(t)$ by the set of transition components $a(n, n-\alpha)e^{i\omega(n,n-\alpha)t}$.
2. Replace $x^2(t)$ with the set $\sum_\alpha a(n, n-\alpha)e^{i\omega(n,n-\alpha)t}a(n-\alpha, n-\beta)e^{i\omega(n-\alpha,n-\beta)t}$.
3. Keep Newton's second law, $\ddot{x} + f(x) = 0$, but replace x as before.

4. Replace the old quantum condition, $nh = \oint m\dot{x}^2 dt$, with $h = 4\pi m\Sigma_\alpha\{|a(n+\alpha,n)|^2\omega(n+\alpha,n) - |a(n,n-\alpha)|^2\omega(n,n-\alpha)\}$.

The quantum mechanics of Born and Jordan consists of five postulates:

1. $\mathbf{q} = (q(nm)e^{2\pi i\nu(nm)t})$, $\mathbf{p} = (p(nm)e^{2\pi i\nu(nm)t})$,
2. $\nu(jk) + \nu(kl) + \nu(lj) = 0$,
3. $\dot{\mathbf{q}} = \partial\mathbf{H}/\partial\mathbf{p}$, $\dot{\mathbf{p}} = -\partial\mathbf{H}/\partial\mathbf{q}$,
4. $E_n = H(nn)$, and
5. $(\mathbf{pq} - \mathbf{qp})_{\text{diagonal}} = h/2\pi i$,

and four theorems

1. $(\mathbf{pq} - \mathbf{qp})_{\text{nondiagonal}} = 0$,
2. $\dot{\mathbf{g}} = (2\pi i/h)(\mathbf{Hg} - \mathbf{gH})$,
3. $\dot{\mathbf{H}} = 0$, and
4. $h\nu(nm) = H(nn) - H(mm)$.

Quantum mechanics evolved at a rapid pace after the papers of Heisenberg and Born–Jordan. Dirac's paper was received on 7 November 1925.[6] Born, Heisenberg, and Jordan's paper was received on 16 November 1925.[5] The first "textbook" on quantum mechanics appeared in 1926.[75] In a series of papers during the spring of 1926, Schrödinger set forth the theory of wave mechanics.[76] In a paper received June 25, 1926 Born introduced the statistical interpretation of the wave function.[77] The Nobel Prize was awarded to Heisenberg in 1932 (delayed until 1933) to Schrödinger and Dirac in 1933, and to Born in 1954.

APPENDIX: HEISENBERG'S FOUR BREAKTHROUGH IDEAS

We divide Heisenberg's paper[2] into four major reinterpretations. For the most part we will preserve Heisenberg's original notation and arguments.

Reinterpretation 1: Position. Heisenberg considered one-dimensional periodic systems. The classical motion of the system (in a stationary state labeled n) is described by the time-dependent position $x(n,t)$.[78] Heisenberg represents this periodic function by the Fourier series

$$x(n,t) = \sum_\alpha a_\alpha(n)e^{i\alpha\omega(n)t}. \tag{A1}$$

Unless otherwise noted, sums over integers go from $-\infty$ to ∞. The αth Fourier component related to the nth stationary state has amplitude $a_\alpha(n)$ and frequency $\alpha\omega(n)$. According to the correspondence principle, the αth Fourier component of the classical motion in the state n corresponds to the quantum jump from state n to state $n-\alpha$.[8,26] Motivated by this principle, Heisenberg replaced the classical component $a_\alpha(n)e^{i\alpha\omega(n)t}$ by the transition component $a(n,n-\alpha)e^{i\omega(n,n-\alpha)t}$.[79] We could say that the Fourier harmonic is replaced by a "Heisenberg harmonic." Unlike the sum over the classical components in Eq. (A1), Heisenberg realized that a similar sum over the transition components is meaningless. Such a quantum Fourier series could not describe the electron motion in one stationary state (n) because each term in the sum describes a transition process associated with two states (n and $n-\alpha$).

Heisenberg's next step was bold and ingenious. Instead of reinterpreting $x(t)$ as a *sum* over transition components, he represented the position by the *set* of transition components. We symbolically denote Heisenberg's reinterpretation as

$$x \rightarrow \{a(n,n-\alpha)e^{i\omega(n,n-\alpha)t}\}. \tag{A2}$$

Equation (A2) is the first breakthrough relation.

Reinterpretation 2: Multiplication. To calculate the energy of a harmonic oscillator, Heisenberg needed to know the quantity x^2. How do you square a set of transition components? Heisenberg posed this fundamental question twice in his paper.[80] His answer gave birth to the algebraic structure of quantum mechanics. We restate Heisenberg's question as "If x is represented by $\{a(n,n-\alpha)e^{i\omega(n,n-\alpha)t}\}$ and x^2 is represented by $\{b(n,n-\beta)e^{i\omega(n,n-\beta)t}\}$, how is $b(n,n-\beta)$ related to $a(n,n-\alpha)$?"

Heisenberg answered this question by reinterpreting the square of a Fourier series with the help of the Ritz principle. He evidently was convinced that quantum multiplication, whatever it looked like, must reduce to Fourier-series multiplication in the classical limit. The square of Eq. (A1) gives

$$x^2(n,t) = \sum_\beta b_\beta(n)e^{i\beta\omega(n)t}, \tag{A3}$$

where the βth Fourier amplitude is

$$b_\beta(n) = \sum_\alpha a_\alpha(n)a_{\beta-\alpha}(n). \tag{A4}$$

In the new quantum theory Heisenberg replaceed Eqs. (A3) and (A4) with

$$x^2 \rightarrow \{b(n,n-\beta)e^{i\omega(n,n-\beta)t}\}, \tag{A5}$$

where the $n \rightarrow n-\beta$ transition amplitude is

$$b(n,n-\beta) = \sum_\alpha a(n,n-\alpha)a(n-\alpha,n-\beta). \tag{A6}$$

In constructing Eq. (A6) Heisenberg uncovered the symbolic algebra of atomic processes.

The logic behind the quantum rule of multiplication can be summarized as follows. Ritz's sum rule for atomic frequencies, $\omega(n,n-\beta) = \omega(n,n-\alpha) + \omega(n-\alpha,n-\beta)$, implies the product rule for Heisenberg's kinematic elements, $e^{i\omega(n,n-\beta)t} = e^{i\omega(n,n-\alpha)t}e^{i\omega(n-\alpha,n-\beta)t}$, which is the backbone of the multiplication rule in Eq. (A6). Equation (A6) allowed Heisenberg to algebraically manipulate the transition components.

Reinterpretation 3: Motion. Equations (A2), (A5), and (A6) represent the new "kinematics" of quantum theory—the new meaning of the position x. Heisenberg next turned his attention to the new "mechanics." The goal of Heisenberg's mechanics is to determine the amplitudes, frequencies, and energies from the given forces. Heisenberg noted that in the old quantum theory $a_\alpha(n)$ and $\omega(n)$ are determined by solving the classical equation of motion

$$\ddot{x} + f(x) = 0, \tag{A7}$$

and quantizing the classical solution—making it depend on n—via the quantum condition

$$\oint m\dot{x}dx = nh. \tag{A8}$$

In Eqs. (A7) and (A8) $f(x)$ is the force (per mass) function and m is the mass.

Heisenberg assumed that Newton's second law in Eq. (A7) is valid in the new quantum theory provided that the classical quantity x is replaced by the set of quantities in Eq. (A2), and $f(x)$ is calculated according to the new rules of amplitude algebra. Keeping the same form of Newton's law of dynamics, but adopting the new kinematic meaning of x is the third Heisenberg breakthrough.

Reinterpretation 4: Quantization. How did Heisenberg reinterpret the old quantization condition in Eq. (A8)? Given the Fourier series in Eq. (A1), the quantization condition, $nh = \oint m\dot{x}^2 dt$, can be expressed in terms of the Fourier parameters $a_\alpha(n)$ and $\omega(n)$ as

$$nh = 2\pi m \sum_\alpha |a_\alpha(n)|^2 \alpha^2 \omega(n). \tag{A9}$$

For Heisenberg, setting $\oint p dx$ equal to an integer multiple of h was an arbitrary rule that did not fit naturally into the dynamical scheme. Because his theory focuses exclusively on transition quantities, Heisenberg needed to translate the old quantum condition that fixes the properties of the states to a new condition that fixes the properties of the transitions between states. Heisenberg believed[14] that what matters is the difference between $\oint p dx$ evaluated for neighboring states: $[\oint p dx]_n - [\oint p dx]_{n-1}$. He therefore took the derivative of Eq. (A9) with respect to n to eliminate the forced n dependence and to produce a differential relation that can be reinterpreted as a difference relation between transition quantities. In short, Heisenberg converted

$$h = 2\pi m \sum_\alpha \alpha \frac{d}{dn} (|a_\alpha(n)|^2 \alpha \omega(n)) \tag{A10}$$

to

$$h = 4\pi m \sum_{\alpha=0}^{\infty} \{|a(n+\alpha,n)|^2 \omega(n+\alpha,n) - |a(n,n-\alpha)|^2 \omega(n,n-\alpha)\}. \tag{A11}$$

In a sense Heisenberg's "amplitude condition" in Eq. (A11) is the counterpart to Bohr's frequency condition (Ritz's frequency combination rule). Heisenberg's condition relates the amplitudes of different lines within an atomic spectrum and Bohr's condition relates the frequencies. Equation (A11) is the fourth Heisenberg breakthrough.[81]

Equations (A7) and (A11) constitute Heisenberg's new mechanics. In principle, these two equations can be solved to find $a(n,n-\alpha)$ and $\omega(n,n-\alpha)$. No one before Heisenberg knew how to calculate the amplitude of a quantum jump. Equations (A2), (A6), (A7), and (A11) define Heisenberg's program for constructing the line spectrum of an atom from the given force on the electron.

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[1] The name "quantum mechanics" appeared for the first time in the literature in M. Born, "Über Quantenmechanik," Z. Phys. **26**, 379–395 (1924).
[2] W. Heisenberg, "Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen," Z. Phys. **33**, 879–893 (1925), translated in Ref. 3, paper 12.
[3] *Sources of Quantum Mechanics*, edited by B. L. van der Waerden (Dover, New York, 1968).
[4] M. Born and P. Jordan, "Zur Quantenmechanik," Z. Phys. **34**, 858–888 (1925); English translation in Ref. 3, paper 13.
[5] M. Born, W. Heisenberg, and P. Jordan, "Zur Quantenmechanik II," Z. Phys. **35**, 557–615 (1926), English translation in Ref. 3, paper 15.
[6] P. A. M. Dirac, "The fundamental equations of quantum mechanics," Proc. R. Soc. London, Ser. A **109**, 642–653 (1925), reprinted in Ref. 3, paper 14.
[7] The name "matrix mechanics" did not appear in the original papers of 1925 and 1926. The new mechanics was most often called "quantum mechanics." At Göttingen, some began to call it "matrix physics." Heisenberg disliked this terminology and tried to eliminate the mathematical term "matrix" from the subject in favor of the physical expression "quantum-theoretical magnitude." [Ref. 17, p. 362]. In his Nobel Lecture delivered 11 December 1933, Heisenberg referred to the two versions of the new mechanics as "quantum mechanics" and "wave mechanics." See *Nobel Lectures in Physics 1922–1941* (Elsevier, Amsterdam, 1965)].
[8] W. A. Fedak and J. J. Prentis, "Quantum jumps and classical harmonics," Am. J. Phys. **70**, 332–344 (2002).
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[14] Duncan, A. and Janssen, M., "On the verge of Umdeutung in Minnesota: Van Vleck and the correspondence principle," Arch. Hist. Exact Sci. **61**, 553–624 (2007).
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[16] G. Birtwistle, *The New Quantum Mechanics* (Cambridge U.P., London, 1928).
[17] C. Jungnickel and R. McCormmach, *Intellectual Mastery of Nature* (University of Chicago Press, Chicago, 1986), Vol. 2.
[18] W. Heisenberg, "Development of concepts in the history of quantum theory," Am. J. Phys. **43**, 389–394 (1975).
[19] M. Bowen and J. Coster, "Born's discovery of the quantum-mechanical matrix calculus," Am. J. Phys. **48**, 491–492 (1980).
[20] M. Born, *My Life: Recollections of a Nobel Laureate* (Taylor & Francis, New York, 1978). Born wrote that (pp. 218–219) "This paper by Jordan and myself contains the formulation of matrix mechanics, the first printed statement of the commutation law, some simple applications to the harmonic and anharmonic oscillator, and another fundamenal idea: the quantization of the electromagnetic field (by regarding the components as matrices). Nowadays, textbooks speak without exception of Heisenberg's matrices, Heisenberg's commutation law and Dirac's field quantization."
[21] In 1928 Einstein nominated Heisenberg, Born, and Jordan for the Nobel Prize [See A. Pais, *Subtle Is the Lord: The Science and the Life of Albert Einstein* (Oxford U.P., New York, 1982), p. 515]. Possible explanations of why Born and Jordan did not receive the Nobel Prize are given in Ref. 10 and Ref. 22, pp. 191–193.
[22] N. Greenspan, *The End of the Certain World: The Life and Science of Max Born* (Basic Books, New York, 2005).
[23] See Ref. 20, p. 220.
[24] E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1998), pp. 320–323.
[25] Reference 11, p. 205.
[26] N. Bohr, "On the quantum theory of line-spectra," reprinted in Ref. 3, paper 3.
[27] Reference 3 p. 276 paper 12.
[28] Reference 20, pp. 217–218.
[29] Reference 20, p. 218.
[30] Reference 3, pp. 277, paper 13.
[31] Reference 3, pp. 277–278, paper 13.
[32] R. L. Liboff, *Introductory Quantum Mechanics* (Addison-Wesley, San Francisco, 2003), Chap. 3; R. Shankar, *Principles of Quantum Mechanics* (Plenum, New York, 1994), Chap. 4; C. Cohen-Tannoudji, B. Diu, and F. Laloë, *Quantum Mechanics* (Wiley, New York, 1977), Chap. III.
[33] Reference 3, p. 287, paper 13.
[34] Reference 12, pp. 217–218.
[35] Reference 3, p. 280, paper 13.
[36] A. Cayley, "Sept différents mémoires d'analyse," Mathematika **50**, 272–

317 (1855); A. Cayley, "A memoir on the theory of matrices," Philos. Trans. R. Soc. London, Ser. A **148**, 17–37 (1858).

[37] The last chapter (Bemerkungen zur Elektrodynamik) is not translated in Ref. 3. See Ref. 13, pp. 87–90 for a discussion of the contents of this section.

[38] In Heisenberg's paper (see Ref. 2) the connection between $|q(nm)|^2$ and transition probability is implied but not discussed. See Ref. 3, pp. 30–32, for a discussion of Heisenberg's assertion that the transition amplitudes determine the transition probabilities. The relation between a squared amplitude and a transition probability originated with Bohr who conjectured that the squared Fourier amplitude of the classical electron motion provides a measure of the transition probability (see Refs. 8 and 26). The correspondence between classical intensities and quantum probabilities was studied by several physicists including H. Kramers, *Intensities of Spectral Lines* (A. F. Host and Sons, Kobenhaven, 1919); R. Ladenburg in Ref. 3, paper 4, and J. H. Van Vleck, "Quantum principles and line spectra," Bulletin of the National Research Council, Washington, DC, 1926, pp. 118–153.

[39] Reference 3, p. 287, paper 13.

[40] W. Ritz, "Über ein neues Gesetz der Serienspektren," Phys. Z. **9**, 521–529 (1908); W. Ritz, "On a new law of series spectra," Astrophys. J. **28**, 237–243 (1908). The Ritz combination principle was crucial in making sense of the regularities in the line spectra of atoms. It was a key principle that guided Bohr in constructing a quantum theory of line spectra. Observations of spectral lines revealed that pairs of line frequencies combine (add) to give the frequency of another line in the spectrum. The Ritz combination rule is $\nu(nk) + \nu(km) = \nu(nm)$, which follows from Eqs. (4) and (7). As a universal, exact law of spectroscopy, the Ritz rule provided a powerful tool to analyze spectra and to discover new lines. Given the measured frequencies ν_1 and ν_2 of two known lines in a spectrum, the Ritz rule told spectroscopists to look for new lines at the frequencies $\nu_1 + \nu_2$ or $\nu_1 - \nu_2$.

[41] In the letter dated 18 September 1925 Heisenberg explained to Pauli that the frequencies ν_{ik} in the Born–Jordan theory obey the "combination relation $\nu_{ik} + \nu_{kl} = \nu_{il}$ or $\nu_{ik} = (W_i - W_k)/h$ but naturally it is *not* to be assumed that W is the energy." See Ref. 3, p. 45.

[42] Reference 3, p. 287, paper 13.

[43] Reference 3, p. 289, paper 13.

[44] Born and Jordan devote a large portion of Chap. 1 to developing a matrix calculus to give meaning to matrix derivatives such as $d\mathbf{q}/dt$ and $\partial\mathbf{H}/\partial\mathbf{p}$. They introduce the process of "symbolic differentiation" for constructing the derivative of a matrix with respect to another matrix. For a discussion of Born and Jordan's matrix calculus, see Ref. 13, pp. 68–71. To deal with arbitrary Hamiltonian functions, Born and Jordan formulated a more general dynamical law by converting the classical action principal, $\int L dt = $extremum, into a quantal action principal, $D(\mathbf{p}\dot{\mathbf{q}} - \mathbf{H}(\mathbf{pq}))$ =extremum, where D denotes the trace (diagonal sum) of the Lagrangian matrix, $\mathbf{p}\dot{\mathbf{q}} - \mathbf{H}$. See Ref. 3, pp. 289–290.

[45] Reference 3, p. 292. This statement by Born and Jordan appears in Sec. IV of their paper following the section on the basic laws. We have included it with the postulates because it is a deep assumption with far-reaching consequences.

[46] In contemporary language the states labeled $n = 0, 1, 2, 3, \ldots$ in Heisenberg's paper and the Born–Jordan paper are exact stationary states (eigenstates of $\mathbf{H}$). The Hamiltonian matrix is automatically a diagonal matrix with respect to this basis.

[47] Although Heisenberg, Born, and Jordan made the "energy of the state" and the "transition between states" rigorous concepts, it was Schrödinger who formalized the concept of the "state" itself. It is interesting to note that "On quantum mechanics II" by Born, Heisenberg, and Jordan was published before Schrödinger and implicitly contains the first mathematical notion of a quantum state. In this paper (Ref. 3, pp. 348–353), each Hermitian matrix **a** is associated with a "bilinear form" $\Sigma_{nm} a(nm) x_n x_m^*$. Furthermore, they identified the "energy spectrum" of a system with the set of "eigenvalues" W in the equation $Wx_k - \Sigma_l H(kl)x_l = 0$. In present-day symbolic language the bilinear form and eigenvalue problem are $\langle\Psi|\mathbf{a}|\Psi\rangle$ and $\mathbf{H}|\Psi\rangle = \mathbf{W}|\Psi\rangle$, respectively, where the variables x_n are the expansion coefficients of the quantum state $|\Psi\rangle$. At the time, they did not realize the physical significance of their eigenvector $(x_1, x_2, \ldots)$ as representing a stationary state.

[48] Reference 3, pp. 290–291, paper 13.

[49] This is the sentence from Born's 1924 paper (See Ref. 1) where the name "quantum mechanics" appears for the first time in the physics literature [Ref. 3, p. 182].

[50] See the chapter "The transition to quantum mechanics" in Ref. 12, pp. 181–198 for applications of "Born's correspondence rule." The most important application was deriving Kramer's dispersion formula. See Ref. 3, papers 6–10 and Ref. 14.

[51] Reference 11, pp. 144–145.

[52] The exact relation between the orbital frequency and the optical frequency is derived as follows. Consider the transition from state n of energy $E(n)$ to state $n - \tau$ of energy $E(n - \tau)$. In the limit $n \gg \tau$, that is, large "orbit" and small "jump," the difference $E(n) - E(n - \tau)$ is equal to the derivative $\tau dE/dn$. Given the old quantum condition $J = nh$, it follows that $dE/dn = hdE/dJ$. Thus for $n \gg \tau$ and $J = nh$, we have the relation $[E(n) - E(n - \tau)]/h = \tau dE/dJ$, or equivalently, $\nu(n, n - \tau) = \tau\nu(n)$. This relation proves an important correspondence theorem: In the limit $n \gg \tau$, the frequency $\nu(n, n - \tau)$ associated with the quantum jump $n \rightarrow n - \tau$ is equal to the frequency $\tau\nu(n)$ associated with the τth harmonic of the classical motion in the state n. See Refs. 8 and 26.

[53] Reference 3, p. 191, paper 7.

[54] Suppose that the number of states is finite and equal to the integer N. Then, according to Eq. (20), the diagonal sum (trace) of $\mathbf{pq} - \mathbf{qp}$ would be $D(\mathbf{pq} - \mathbf{qp}) = Nh/2\pi i$. This nonzero value of the trace contradicts the purely mathematical relation $D(\mathbf{pq} - \mathbf{qp}) = 0$, which must be obeyed by all finite matrices.

[55] Heisenberg interview quoted in Ref. 12, p. 281, footnote 45.

[56] Reference 17, p. 361.

[57] Reference 3, p. 288, paper 13. The name "Diagonality theorem" is ours. The condition $\nu(nm) \neq 0$ when $n \neq m$ implies that the system is nondegenerate.

[58] In contemporary language a conserved quantity is an operator that commutes with the Hamiltonian operator $\mathbf{H}$. For such commuting operators there exists a common set of eigenvectors. In the energy eigenbasis that underlies the Born–Jordan formulation, the matrices representing $\mathbf{H}$ and all conserved quantities are automatically diagonal.

[59] Born and Jordan's proof that Eq. (24) vanishes is based on a purely mathematical property of "symbolic differentiation" discussed in Sec. II of their paper (See Ref. 4). For a separable Hamiltonian of the form $\mathbf{H} = \mathbf{p}^2/2m + \mathbf{U}(\mathbf{q})$, the proof is simpler. For this case Eq. (24) becomes $\dot{\mathbf{d}} = \mathbf{q}(\partial\mathbf{U}/\partial\mathbf{q}) - (\partial\mathbf{U}/\partial\mathbf{q})\mathbf{q} + \mathbf{p}(\mathbf{p}/m) - (\mathbf{p}/m)\mathbf{p}$. Because $\mathbf{p}$ and $\mathbf{q}$ are separated in this expression, we do not have to consider the inequality $\mathbf{pq} \neq \mathbf{qp}$. The expression reduces to $\dot{\mathbf{d}} = 0$.

[60] Reference 3, p. 292, paper 13. In Ref. 4, Born and Jordan refer to $\mathbf{pq} - \mathbf{qp} = (h/2\pi i)\mathbf{1}$ as the "verschärfte Quantenbedingung," which has been translated as "sharpened quantum condition" (Ref. 13, p. 77), "stronger quantum condition" (Ref. 3, p. 292), and "exact quantum condition" (Ref. 12, p. 220).

[61] J. J. Sakurai, *Modern Quantum Mechanics* (Addison-Wesley, San Francisco, 1994), pp. 83–84; A. Messiah, *Quantum Mechanics* (J Wiley, New York, 1958), Vol. I, p. 316.

[62] Reference 3, p. 293, paper 13.

[63] Proving the frequency condition—the second general principle of Bohr—was especially important because this purely quantal condition was generally regarded as a safely established part of physics. Prior to Born and Jordan's mechanical proof of the frequency condition, there existed a "thermal proof" given by Einstein in his historic paper, "On the quantum theory of radiation," Phys. Z. **18**, 121 (1917), translated in Ref. 3, pp. 63–77. In this paper Einstein provides a completely new derivation of Planck's thermal radiation law by introducing the notion of transition probabilities (A and B coefficients). Bohr's frequency condition emerges as the condition necessary to reduce the Boltzmann factor $\exp[(E_n - E_m)/kT]$ in Einstein's formula to the "Wien factor" $\exp(h\nu/kT)$ in Planck's formula.

[64] Reference 3, p. 291, paper 13.

[65] Reference 3, pp. 291–292, paper 13. Born and Jordan do not refer to the consequences in Eqs. (37) and (38) as theorems. The label "Energy theorems" is ours.

[66] Instead of postulating the equations of motion and deriving the energy theorems, we could invert the proof and postulate the energy theorems and derive the equations of motion. This alternate logic is mentioned in Ref. 3, p. 296 and formalized in Ref. 5 (Ref. 3, p. 329). Also see J. H. Van Vleck, "Note on the postulates of the matrix quantum dynamics," Proc. Natl. Acad. Sci. U.S.A. **12**, 385–388 (1926).

[67] Reference 3, pp. 293–294, paper 13. The proof of the energy theorems was based on separable Hamiltonians defined in Eq. (29). To generalize the proof Born and Jordan consider more general Hamiltonian functions

H(**pq**) and discover the need to symmetrize the functions. For example, for $\mathbf{H}^*=\mathbf{p}^2\mathbf{q}$, it does not follow that $\dot{\mathbf{H}}^*=0$. However, they note that $\mathbf{H}=(\mathbf{p}^2\mathbf{q}+\mathbf{q}\mathbf{p}^2)/2$ yields the same equations of motion as $\mathbf{H}^*$ and also conserves energy, $\dot{\mathbf{H}}=0$. The symmetrization rule reflects the noncommutativity of **p** and **q**.

[68] In the Heisenberg, Born–Jordan approach the transition components of the "matter variables" **q** and **p** are simply assumed to oscillate in time with the radiation frequencies. In contemporary texts a rigorous proof of Bohr's frequency condition involves an analysis of the interaction between matter and radiation (radiative transitions) using time-dependent perturbation theory. See Ref. 24, Chap. 19.

[69] Reference 3, p. 292, paper 13.

[70] Using the language of state vectors and bra-kets, the matrix element of an operator **g** is $g_{nm}(t)=\langle\Psi_n(t)|\mathbf{g}|\Psi_m(t)\rangle$, where the energy eigenstate is $|\Psi_n(t)\rangle=\exp(-2\pi iE_nt/h)|\Psi_n(0)\rangle$. This Schrödinger element is equivalent to the Born–Jordan element in Eq. (44).

[71] Reference 3, p. 279, paper 13. Heisenberg was able to demonstrate energy conservation and Bohr's frequency condition for two systems (anharmonic oscillator and rotator). The anharmonic oscillator analysis was limited to second-order perturbation theory.

[72] Reference 3. Born and Jordan do not pursue this direct method of proof noting that for the most general Hamiltonians the calculation "becomes so exceedingly involved that it seems hardly feasible." (Ref. 3, p. 296). In a footnote on p. 296, they note that for the special case $\mathbf{H}=\mathbf{p}^2/2m+U(\mathbf{q})$, the proof can be carried out immediately. The details of this proof can be found in Ref. 73.

[73] J. J. Prentis and W. A. Fedak, "Energy conservation in quantum mechanics," Am. J. Phys. **72**, 580–590 (2004).

[74] Reference 3, p. 296, paper 13.

[75] M. Born, *Problems of Atomic Dynamics* (MIT Press, Cambridge, 1970).

[76] E. Schrödinger, *Collected Papers on Wave Mechanics* (Chelsea, New York, 1978).

[77] M. Born, "Zur Quantenmechanik der Stoßvorgänge," Z. Phys. **37**, 863–867 (1926).

[78] Heisenberg's "classical" quantity $x(n,t)$ is the classical solution $x(t)$ of Newton's equation of motion subject to the old quantum condition $\oint m\dot{x}dx=nh$. For example, given the purely classical position function $x(t)=a\cos\omega t$ of a harmonic oscillator, the condition $\oint m\dot{x}^2dt=nh$ quantizes the amplitude, making a depend on n as follows: $a(n)=\sqrt{nh/\pi m\omega}$. Thus, the motion of the harmonic oscillator in the stationary state n is described by $x(n,t)=\sqrt{nh/\pi m\omega}\cos\omega t$.

[79] The introduction of transition components $a(n,n-\tau)e^{i\omega(n,n-\alpha)t}$ into the formalism was a milestone in the development of quantum theory. The one-line abstract of Heisenberg's paper reads "The present paper seeks to establish a basis for theoretical quantum mechanics founded exclusively upon relationships between quantities which in principle are observable" (Ref. 3, p. 261). For Heisenberg, the observable quantities were $a(n,n-\tau)$ and $\omega(n,n-\tau)$, that is, the amplitudes and the frequencies of the spectral lines. Prior to 1925, little was known about transition amplitudes. There was a sense that Einstein's transition probabilities were related to the squares of the transition amplitudes. Heisenberg made the transition amplitudes (and frequencies) the central quantities of his theory. He discovered how to manipulate them, relate them, and calculate their values.

[80] Reference 3, pp. 263–264, paper 12.

[81] Heisenberg notes (Ref. 3, p. 268, paper 12) that Eq. (A11) is equivalent to the sum rule of Kuhn and Thomas (Ref. 3, paper 11). For a discussion of Heisenberg's development of the quantum condition, see Mehra and H. Rechenberg, *The Historical Development of Quantum Theory* (Springer, New York, 1982), Vol. 2, pp. 243–245, and Ref. 14.

SCIENTIFIC APTITUDE AND AUTISM

There's even some evidence that scientific abilities are associated with traits characteristic of autism, the psychological disorder whose symptoms include difficulties in social relationships and communication, or its milder version, Asperger syndrome. One recent study, for instance, examined different groups according to the Autism-Spectrum Quotient test, which measures autistic traits. Scientists scored higher than nonscientists on this test, and within the sciences, mathematicians, physical scientists, and engineers scored higher than biomedical scientists.

Sidney Perkowitz, *Hollywood Science: Movies, Science, and the End of the World* (Columbia University Press, 2007), p. 170.