

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

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Abstract

In July 1925 Heisenberg published a paper [Z. Phys. **33** 879-893 (1925)] which ended the period of 'the Old Quantum Theory' and ushered in the new era of Quantum Mechanics. This epoch-making paper is generally regarded as being difficult to follow, perhaps partly because Heisenberg provided few clues as to how he arrived at the results which he reported. Here we give details of calculations of the type which, we suggest, Heisenberg may have performed. We take as a specific example 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. We emphasize that the results are precisely those obtained in standard quantum mechanics, and suggest that some discussion of the approach - based on the direct computation of transition amplitudes - could usefully be included in undergraduate courses on quantum mechanics.

1 Introduction

Heisenberg's paper of July 1925¹, entitled 'Quantum-mechanical re-interpretation of kinematic and mechanical relations'^{2,3}, was the breakthrough which quickly led to the first complete formulations of quantum mechanics^{4,5,6}. Despite its undoubtedly crucial historical role, Heisenberg's paper is not generally referred

to in undergraduate courses on quantum mechanics - in contrast, say, to the place of Einstein's 1905 paper in the teaching of Relativity. Indeed it is still widely regarded as being difficult to understand and - perhaps because of this - of only historical interest today. For example, Weinberg⁷ has written as follows:

'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 that sense, Heisenberg's 1925 paper was pure magic.

Perhaps we should not look too closely at Heisenberg's first paper.....'

There have, in fact, been many discussions aimed at elucidating the main ideas in Heisenberg's paper, of which Refs 3, 8, 9-18 no doubt represent only a partial selection; of these the most detailed appear to be Ref. 3 pages 28-35, Ref. 8 pages 204-224, Ref. 10 pages 161-188, and Ref. 11 chapter IV. Of course, it may well not be possible ever to render completely comprehensible the mysterious processes whereby magician-physicists 'jump over all intermediate steps to a new insight about nature'¹⁹. In our opinion, however, one of the main barriers to understanding Heisenberg's paper, for most people, is a more prosaic one: namely, that he gives remarkably few details of the calculations he actually performed, in order to arrive at his results for the one-dimensional model systems which he treats (anharmonic oscillators and the rigid rotator).

One aim of the present paper is therefore to make Heisenberg's paper more accessible to scientists, and to historians of science, by briefly reviewing the line of reasoning he followed in setting up his new calculational scheme (section 2), and then by presenting (in section 3) full details of a calculation typical of those we conjecture that Heisenberg himself performed. Our 'reconstruction' is based on the assumption that, having formulated a scheme which was capable in principle of determining uniquely the relevant physical quantities (transition frequencies and amplitudes), Heisenberg then applied it rigorously to various 'toy' mechanical systems, without any further recourse to the kind of 'inspired guesswork' that characterised the Old Quantum Theory. Surprisingly, this point of view appears to be novel: MacKinnon¹⁰, and Mehra and Rechenberg¹¹, for example, consider that Heisenberg arrived at the crucial recursion relations (equations (40) - (43) below), in the quantum case, by essentially guessing the appropriate generalisation of their classical counterparts (see section 3). We are unaware of any evidence, now, 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 scheme, the results of applying which are precisely those of standard quantum mechanics. Thus a second aim of our paper is to stress both the correctness and the practicality of what we conjecture to be Heisenberg's calculational scheme, and to stimulate a re-appraisal of the possibility of including at least some discussion of it in undergraduate

courses.

2 Heisenberg's ‘transition amplitude’ approach

2.1 Quantum kinematics

As is well known, Heisenberg begins his paper with a programmatic call to ‘discard all hope of observing hitherto unobservable quantities, such as the position and period of the electron’²⁰, 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 points to the energies $W(n)$ of the (Bohr) stationary states, together with the associated (Einstein-Bohr) frequencies²¹

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

noting that these frequencies, which characterise radiation emitted in the transition $n \rightarrow n - \alpha$, depend on two variables. An example of something he wishes to exclude from the new theory is the time-dependent position coordinate $x(t)$. In considering what might replace it, he turns 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 in fact the type of system studied by Heisenberg. For a state characterised by the label n , fundamental frequency $\omega(n)$ and coordinate $x(n, t)$, one can represent $x(n, t)$ as a Fourier series

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

According to classical theory, the energy emitted per unit time (that is, the power) in a transition corresponding to the α th harmonic $\omega(n)\alpha$ is²²

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

In the quantum theory, however, the transition frequency corresponding to the classical ‘ $\omega(n)\alpha$ ’ is in general *not* a simple multiple of a fundamental frequency, but is given by (1): thus $\omega(n)\alpha$ is replaced by $\omega(n, n - \alpha)$. Correspondingly, Heisenberg introduces the quantum analogue of $X_{\alpha}(n)$, which he writes as $X(n, n - \alpha)$ ²⁴. Further, the left hand side of (3) has, in the quantum theory, 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 (3) becomes

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

It is the *transition amplitudes* $X(n, n - \alpha)$ which Heisenberg fastens upon as being satisfactorily ‘observable’; like the transition frequencies, they depend on two discrete variables²⁵.

Equation (4) refers, however, to only one specific transition. For a full description of atomic dynamics (as then conceived), one will need to consider all the quantities $X(n, n - \alpha)\exp[i\omega(n, n - \alpha)t]$. In the classical case, the terms $X_\alpha(n)\exp[i\omega(n)\alpha t]$ may be combined to yield $x(t)$ via (2). But in the quantum theory, Heisenberg says, 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 α [i.e. in the amplitude $X(n, n - \alpha)$ and frequency $\omega(n, n - \alpha)$].’ ‘However’, he continues, ‘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 $x(t) \dots$ ’ This is the first of Heisenberg’s ‘magical jumps’ - and certainly a very large one. Representing $x(t)$ in this way seems to be the sense in which he considered himself to be ‘re-interpreting the kinematics’.

Still concerned with the kinematics, Heisenberg immediately poses the question: ‘how is the quantity $x(t)^2$ to be represented?’ In classical theory, the answer is straightforward. From (2) we obtain

$$[x(t)]^2 = \sum_{\alpha} \sum_{\gamma} X_{\alpha}(n) X_{\gamma}(n) e^{i\omega(n)(\alpha+\gamma)t}. \quad (5)$$

Relabelling $\alpha + \gamma$ as β , (5) becomes

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

where

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

Thus classically $[x(t)]^2$ is represented (via a Fourier series) by the set of quantities $Y_{\beta}(n)\exp[i\omega(n)\beta t]$, the frequency $\omega(n)\beta$ being the simple combination $[\omega(n)\alpha + \omega(n)(\beta - \alpha)]$. 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 (7)?

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

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

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

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

Cancelling the exponentials on both sides of (9) we are left with

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

which is Heisenberg's law for multiplying transition amplitudes together.

He indicates the simple extension of the rule to higher powers $[x(t)]^n$, but at once notices that a 'significant difficulty arises, however, if we consider two quantities $x(t), y(t)$ and ask after their product $x(t)y(t) \dots$. 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'. This 'difficulty' clearly unsettled Heisenberg: but it very quickly became clear that the *non-commutativity* (in general) of kinematical quantities in quantum theory was the really essential new technical idea in the paper. Born recognised (10) as matrix multiplication (something unknown to Heisenberg in July 1925), and he and Jordan rapidly produced Ref. 4, the first paper to state the fundamental commutation relation (in modern notation)

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

Dirac's paper followed soon after⁵, and then the 'three-man' paper of Born, Heisenberg and Jordan⁶.

The economy and force of Heisenberg's argument in reaching (10) is surely very remarkable - and it seems at least worth considering whether presenting it to undergraduates might not help them to understand the 'almost necessity' of non-commuting quantities in quantum theory.

2.2 Quantum dynamics

Having identified the transition amplitudes $X(n, n - \alpha)$ and frequencies $\omega(n, n - \alpha)$ as the 'observables' with which the new theory should deal, Heisenberg now turns his attention to how they may be determined 'from the given forces of the system' - that is, by the dynamics. In the Old Quantum Theory, he notes, this would be done in two stages: (a) by integration of the equation of motion

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

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

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

where the integral is to be evaluated over one period of the motion. As regards (12), Heisenberg says that it is 'very natural' to take over the classical equation of motion into quantum theory, replacing the classical quantities $x(t)$ and $f(x)$ by their kinematical re-interpretations²⁶, as in the previous section (or, as we would say today, by taking matrix elements of the operator equation of motion $\ddot{\hat{x}} + f(\hat{x}) = 0$). He notes that in the classical case a solution can be obtained by expressing $x(t)$ as a Fourier series, insertion of which into the equation of

motion leads (in simple special cases) to a set of recursion relations for the Fourier coefficients. In the quantum theory, Heisenberg says, ‘we are at present forced to adopt this way of solving equation (12) [his equation H(11)]....since it was not possible to define a quantum-theoretical function analogous to the [classical] function $x(n, t)$.’ In section 3 we shall consider the simple example (the first of those chosen by Heisenberg) $f(x) = \omega_0^2 x + \lambda x^2$, obtaining the appropriate recursion relations in both the classical and the quantum cases.

A ‘quantum-theoretical re-interpretation’ of (13) is now required, in terms of the transition amplitudes $X(n, n - \alpha)$. In the classical case, insertion of (2) into (13) gives

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

using $X_{\alpha}(n) = [X_{-\alpha}(n)]^*$; (14) is H(14). Heisenberg argues that (14) does not sit well with the Correspondence Principle, since the latter should only determine J up to an additive constant (times h). Setting (14) equal to nh , he converts it to the form (H(15))

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

which determines the $X_{\alpha}(n)$ ’s only to within a constant; 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 now replaces the differential in (15) by a *difference*, giving

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

which is H(16)²⁷. As he later recalled, he had noticed that ‘if I wrote down this [presumably (15) above] and tried to translate it according to the scheme of dispersion theory, I got the Thomas-Kuhn sum rule [which is equation (16)]^{28,29}. And that is the point. Then I thought, “That is apparently how it is done”³⁰.

By ‘the scheme of dispersion theory’, Heisenberg is referring to what Jammer³¹ calls Born’s correspondence rule, namely³²

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

or rather to its iteration in the form³³

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

as used in the Kramers-Heisenberg theory of dispersion^{34,35}. It took Born only a few days to show that Heisenberg’s quantum condition (16) was in fact the diagonal matrix element of (11), and to guess³⁶ that the off-diagonal elements of

$\hat{x}\hat{p}-\hat{p}\hat{x}$ were zero, a result which was shown to be compatible with the equations of motion in Born and Jordan's paper⁴.

At this point, when we have momentarily advanced a little beyond July 1925, it may be appropriate to emphasize that Heisenberg's transition amplitude $X(n, n-\alpha)$ is indeed precisely the same as the quantum-mechanical matrix element $\langle n-\alpha|\hat{x}|n\rangle$, where $|n\rangle$ is the exact eigenstate with energy $W(n)$. The relation of (16) to the fundamental commutator (11) is briefly recalled in Appendix A.

Returning to the development of Heisenberg's paper, he summarizes the state of affairs reached so far by the statement that equations (12) and (16) 'if soluble, contain a complete determination not only of the frequencies and energies, but also of the quantum theoretical transition probabilities'. We draw attention to the strong claim here: that he has arrived at a new *calculational scheme*, which will *completely determine* the *observable quantities*. Let us now see in detail how this scheme works, for the case of a harmonic oscillator perturbed by an anharmonic force of the form λx^2 per unit mass³⁷.

3 Heisenberg's calculational scheme, and its detailed working-out for the ' λx^2 ' anharmonic oscillator

3.1 Recursion relations in the quantum case

The classical (and, by assumption, quantum-mechanical) equation of motion is

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

Departing now from the order of Heisenberg's presentation, we shall begin by showing how - as he states - (19) leads to recursion relations for the transition amplitudes $X(n, n-\alpha)$. The $(n, n-\alpha)$ representative of the first two terms in (19) is straightforward, being just

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

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

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

The $(n, n-\alpha)$ representative³⁸ of (19) therefore yields³⁹

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

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

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

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

3.2 Perturbation theory

To make the presentation self-contained, we need to include a certain number of ancillary results. Heisenberg begins by considering the perturbative solution of the classical equation (12). He writes the solution in the form

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

where the coefficients a_α , and ω , are themselves to be expanded as a power series in λ , the first terms of which are independent of λ ³⁸:

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

$$a_1 = a_1^{(0)} + \lambda a_1^{(1)} + \lambda^2 a_1^{(2)} + \dots \quad (26)$$

and so on, and

$$\omega = \omega_0 + \lambda \omega^{(1)} + \lambda^2 \omega^{(2)} + \dots \quad (27)$$

Straightforwardly inserting (24) into (12), using standard trigonometric identities, and equating to zero the terms which are constant, and which multiply $\cos \omega t$, $\cos 2\omega t$, etc, one obtains

$$(\text{constant}) \quad \lambda \{ \omega_0^2 a_0 + \frac{1}{2} a_1^2 + [\lambda^2 (a_0^2 + \frac{1}{2} a_2^2) + \dots] \} = 0 \quad (28)$$

$$(\cos \omega t) \quad (-\omega^2 + \omega_0^2) a_1 + [\lambda^2 (a_1 a_2 + 2a_0 a_1) + \dots] = 0 \quad (29)$$

$$(\cos 2\omega t) \quad \lambda \{ (-4\omega^2 + \omega_0^2) a_2 + \frac{1}{2} a_1^2 + [\lambda^2 (a_1 a_3 + 2a_0 a_2) + \dots] \} = 0 \quad (30)$$

$$(\cos 3\omega t) \quad \lambda^2 \{ (-9\omega^2 + \omega_0^2) a_3 + a_1 a_2 + [\lambda^2 (a_1 a_4 + 2a_0 a_3) + \dots] \} = 0 \quad (31)$$

and so on, where the dots stand for higher powers of λ . Dropping all the terms multiplying λ^2 (and higher powers), (28) - (31) become (for $\lambda \neq 0$ and $a_1 \neq 0$)

$$\omega_0^2 a_0 + \frac{1}{2} a_1^2 = 0 \quad (32)$$

$$(-\omega^2 + \omega_0^2) = 0 \quad (33)$$

$$(-4\omega^2 + \omega_0^2) a_2 + \frac{1}{2} a_1^2 = 0 \quad (34)$$

$$(-9\omega^2 + \omega_0^2) a_3 + a_1 a_2 = 0 \quad (35)$$

which are the same as H(18)⁴¹. The ‘lowest order in λ ’ solution is now obtained from (32) - (35) by setting $\omega = \omega_0$, and replacing each a_α by the corresponding one with a superscript ‘⁽⁰⁾’ (c.f. (25), (26)).

Turning now to the quantum case, Heisenberg proposes to seek a solution analogous to (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 away 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 suggests that, in the quantum case, $x(t)$ should be represented by terms of the form

$$\begin{aligned} &\lambda a(n, n), \quad a(n, n - 1) \cos \omega(n, n - 1)t, \quad \lambda a(n, n - 2) \cos \omega(n, n - 2)t, \dots, \\ &\lambda^{\alpha-1} a(n, n - \alpha) \cos \omega(n, n - \alpha)t, \dots, \end{aligned} \quad (36)$$

where, as in (25) - (27),

$$a(n, n) = a^{(0)}(n, n) + \lambda a^{(1)}(n, n) + \lambda^2 a^{(2)}(n, n) + \dots \quad (37)$$

$$a(n, n - 1) = a^{(0)}(n, n - 1) + \lambda a^{(1)}(n, n - 1) + \lambda^2 a^{(2)}(n, n - 1) + \dots \quad (38)$$

and so on, and

$$\omega(n, n - \alpha) = \omega^{(0)}(n, n - \alpha) + \lambda \omega^{(1)}(n, n - \alpha) + \lambda^2 \omega^{(2)}(n, n - \alpha) + \dots \quad (39)$$

As Born and Jordan pointed out⁴, some use of ‘correspondence’ arguments has been made here, in assuming that, as $\lambda \rightarrow 0$, only transitions between adjacent states are possible (we shall return to this point in section 3.3).

Heisenberg now simply *writes down* what he asserts to be the quantum versions of (32) - (35), namely⁴²

$$\omega_0^2 a(n, n) + \frac{1}{4}[a^2(n + 1, n) + a^2(n, n - 1)] = 0 \quad (40)$$

$$-\omega^2(n, n - 1) + \omega_0^2 = 0 \quad (41)$$

$$[-\omega^2(n, n - 2) + \omega_0^2]a(n, n - 2) + \frac{1}{2}[a(n, n - 1)a(n - 1, n - 2)] = 0 \quad (42)$$

$$\begin{aligned} &[-\omega^2(n, n - 3) + \omega_0^2]a(n, n - 3) + \frac{1}{2}[a(n, n - 1)a(n - 1, n - 3) \\ &+ a(n, n - 2)a(n - 2, n - 3)] = 0. \end{aligned} \quad (43)$$

The question we now want to address is: how did Heisenberg arrive at equations (40) - (43)?

Tomonaga⁸, having derived (22), then proceeds to discuss only the $\lambda \rightarrow 0$ limit - i.e. the simple harmonic oscillator, a special case to which we shall return. The only other authors, to our knowledge, who have offered a discussion of the presumed details of Heisenberg’s calculations are⁴³ Mehra and Rechenberg¹¹. They suggest that Heisenberg guessed how to ‘translate’, ‘re-interpret’ or ‘re-formulate’ (their words) the classical equations (32) - (35) into the quantum ones (40) - (43), in a way that was consistent with his multiplication law (10). Although such ‘inspired guesswork’ was undoubtedly necessary in the stages leading up to Heisenberg’s paper of July 1925, to us it seems more plausible that by the time of the paper’s final formulation, Heisenberg realised that he

had a calculational scheme in which guesswork was no longer necessary, and in which (40) - (43), in particular, could be derived.

Unfortunately, we know of no documentary evidence which can directly prove (or disprove) this suggestion. But we think there is some internal evidence for it. In the passage to which attention was drawn earlier, Heisenberg firmly asserts that the formalism he has set up constitutes a complete scheme for calculating everything that needs to be calculated. It is hard to believe that Heisenberg did not realise that it led directly to equations (40) - (43), without the need for any 'translations' of the classical relations (of course, the latter were a nice check on the reasonableness of the quantum relations). At all events, it is the case that (40) - (43) can be straightforwardly derived, as we shall now see.

In order to apply the ansatz (36) to (22), we need to relate the amplitudes $X(n, n - \alpha)$ to the corresponding quantities $\lambda^{\alpha-1}a(n, n - \alpha)$. We first note that in the classical case

$$X_\alpha(n) = X_{-\alpha}^*(n) \quad (44)$$

since $x(t)$ in (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 (44) is $X(n, n - \alpha)$, while that of the right hand side is $X^*(n - \alpha, n)$ (see Ref. 24). Hence the quantum-theoretical analogue of (44) is

$$X(n, n - \alpha) = X^*(n - \alpha, n), \quad (45)$$

which of course 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 he twice discusses 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 (24), and the corresponding quantum terms (36), the $X(n, n - \alpha)$'s should be chosen to be real, so that (45) becomes

$$X(n, n - \alpha) = X(n - \alpha, n) \quad (46)$$

- that is, the matrix with elements $\{X(n, n - \alpha)\}$ is symmetric. Consider now a typical term of (36)

$$\begin{aligned} & \lambda^{\alpha-1}a(n, n - \alpha) \cos[\omega(n, n - \alpha)t] \\ &= \frac{\lambda^{\alpha-1}}{2}a(n, n - \alpha) \{ \exp[i\omega(n, n - \alpha)t] + \exp[-i\omega(n, n - \alpha)t] \} = \\ &= \frac{\lambda^{\alpha-1}}{2}a(n, n - \alpha) \{ \exp[i\omega(n, n - \alpha)t] + \exp[i\omega(n - \alpha, n)t] \} \end{aligned} \quad (47)$$

using $\omega(n, n - \alpha) = -\omega(n - \alpha, n)$ from (1). Assuming that $a(n, n - \alpha) = a(n - \alpha, n)$ as discussed for (46), we see that it is consistent to write

$$X(n, n - \alpha) = \frac{\lambda^{\alpha-1}}{2}a(n, n - \alpha) \quad (48)$$

for positive values of α , and in general

$$X(n, n - \alpha) = \frac{\lambda^{|\alpha|-1}}{2}a(n, n - \alpha), \quad \alpha \neq 0. \quad (49)$$

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

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

For $\alpha = 0$ we obtain

$$\begin{aligned} & \lambda \{ \omega_0^2 a(n, n) + \frac{1}{4} [a^2(n+1, n) + a^2(n, n-1)] + \\ & \lambda^2 [a^2(n, n) + \frac{1}{4} (a^2(n+2, n) + a^2(n, n-2))] \} = 0. \end{aligned} \quad (50)$$

We note the connection with (28), and that (50) reduces to Heisenberg's (40) when the λ^2 term is dropped. Similarly, for $\alpha = 1$ we obtain

$$\begin{aligned} & (-\omega^2(n, n-1) + \omega_0^2) a(n, n-1) + \lambda^2 \{ a(n, n) a(n, n-1) + a(n, n-1) a(n-1, n-1) + \\ & \frac{1}{2} [a(n, n+1) a(n+1, n-1) + a(n, n-2) a(n-2, n-1)] \} = 0 \end{aligned} \quad (51)$$

(c.f. (29)); for $\alpha = 2$

$$\begin{aligned} & \lambda \{ (-\omega^2(n, n-2) + \omega_0^2) a(n, n-2) + \frac{1}{2} a(n, n-1) a(n-1, n-2) + \\ & \lambda^2 [a(n, n) a(n, n-2) + a(n, n-2) a(n-2, n-2) + \frac{1}{2} a(n, n+1) a(n+1, n-2) \\ & + \frac{1}{2} a(n, n-3) a(n-3, n-2)] \} = 0 \end{aligned} \quad (52)$$

(c.f. (30)); and for $\alpha = 3$ (c.f. (31))

$$\begin{aligned} & \lambda^2 \{ (-\omega^2(n, n-3) + \omega_0^2) a(n, n-3) + \\ & \frac{1}{2} [a(n, n-1) a(n-1, n-3) + a(n, n-2) a(n-2, n-3)] + \\ & \lambda^2 [a(n, n) a(n, n-3) + a(n, n-3) a(n-3, n-3) + \frac{1}{2} a(n, n+1) a(n+1, n-3) + \\ & \frac{1}{2} a(n, n-4) a(n-4, n-3)] \} = 0. \end{aligned} \quad (53)$$

On dropping the terms multiplied by λ^2 , (50) - (53) reduce to Heisenberg's (40) - (43). This appears to be the first published derivation of these equations.

In addition to these recurrence relations which follow from the equations of motion, we also need the perturbative version of the quantum condition (16)⁴⁴. Including terms with a λ^2 power, consistent with (50) - (53), (16) becomes

$$\begin{aligned} & \frac{h}{\pi m} = a^2(n+1, n) \omega(n+1, n) - a^2(n, n-1) \omega(n, n-1) \\ & + \lambda^2 [a^2(n+2, n) \omega(n+2, n) - a^2(n, n-2) \omega(n, n-2)]. \end{aligned} \quad (54)$$

We are now ready to obtain the solutions.

3.3 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 equations (50) - (54), and all quantities (a 's and ω 's) are replaced by the corresponding ones with a superscript (0) (c.f. (37) - (39)⁴⁵. In this case, (51) reduces to

$$[-(\omega^{(0)}(n, n-1))^2 + \omega_0^2]a^{(0)}(n, n-1) = 0, \quad (55)$$

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

$$\omega^{(0)}(n, n-1) = \omega_0 \quad (56)$$

for all n . Substituting (56) into the lowest-order version of (54) we find

$$\frac{h}{\pi m \omega_0} = [a^{(0)}(n+1, n)]^2 - [a^{(0)}(n, n-1)]^2. \quad (57)$$

The solution of this difference equation is

$$[a^{(0)}(n, n-1)]^2 = \frac{h}{\pi m \omega_0} (n + \text{constant}), \quad (58)$$

as given in H(20)⁴⁵. To determine the value of the constant, Heisenberg used the idea that in the ground state there can be no transition to a lower state. Thus

$$[a^{(0)}(0, -1)]^2 = 0 \quad (59)$$

and the constant is determined to be zero. This then gives (up to a convention as to sign)

$$a^{(0)}(n, n-1) = \beta \sqrt{n} \quad (60)$$

where

$$\beta = (h/\pi m \omega_0)^{1/2}. \quad (61)$$

Equations (56) and (60) are Heisenberg's first results, and they are in fact appropriate to the simple (unperturbed) oscillator. We can check (60) against standard quantum mechanics via

$$a^{(0)}(n, n-1) = 2X^{(0)}(n, n-1) = 2 {}_0\langle n-1 | \hat{x} | n \rangle_0 \quad (62)$$

where the states $|n\rangle_0$ are unperturbed oscillator eigenstates. It is well known that⁴⁶

$${}_0\langle n-1 | \hat{x} | n \rangle_0 = \left(\frac{\hbar}{2m\omega_0} \right)^{1/2} \sqrt{n} \quad (63)$$

which agrees with (60), using (61). A similar treatment of (50) leads to

$$a^{(0)}(n, n) = -\frac{\beta^2}{4\omega_0^2} (2n+1). \quad (64)$$

Turning next to equation (52), the lowest-order form is

$$(-[\omega^{(0)}(n, n-2)]^2 + \omega_0^2)a^{(0)}(n, n-2) + \frac{1}{2}a^{(0)}(n, n-1)a^{(0)}(n-1, n-2) = 0. \quad (65)$$

Now the composition law must be true for the lowest-order frequencies, so we have

$$\begin{aligned} \omega^{(0)}(n, n-2) &= \omega^{(0)}(n, n-1) + \omega^{(0)}(n-1, n-2) \\ &= 2\omega_0 \end{aligned} \quad (66)$$

using (56), and in general

$$\omega^{(0)}(n, n-\alpha) = \alpha\omega_0 \quad (\alpha = 1, 2, 3, \dots). \quad (67)$$

Using (60), (66) and (67) we then obtain

$$a^{(0)}(n, n-2) = \frac{\beta^2}{6\omega_0^2} \sqrt{n(n-1)}. \quad (68)$$

A similar treatment of (53) yields

$$a^{(0)}(n, n-3) = \frac{\beta^3}{48\omega_0^4} \sqrt{n(n-1)(n-2)}. \quad (69)$$

Consideration of the general lowest-order term in (22) shows that

$$a^{(0)}(n, n-\alpha) = A_\alpha \frac{\beta^\alpha}{\omega_0^{2(\alpha-1)}} \sqrt{\frac{n!}{(n-\alpha)!}}, \quad (70)$$

where A_α is a numerical factor depending on α ; (70) is equivalent to H(21).

At this stage it is instructive to comment briefly on the relation of the above results to those which would be obtained in standard quantum-mechanical perturbation theory. At first sight, it is surprising to see non-zero amplitudes for two-quantum ((68)), three-quantum ((69)) or α -quantum ((70)) transitions appearing at ‘lowest order’. But we have to remember that in Heisenberg’s perturbative ansatz (36), the α -quantum amplitude appears multiplied by a factor $\lambda^{\alpha-1}$. Thus, for example, the ‘lowest order’ two-quantum amplitude is really $\lambda a^{(0)}(n, n-2)$, not just $a^{(0)}(n, n-2)$. Indeed, such a transition is to be expected precisely at order λ^1 , in conventional perturbation theory. The amplitude is $\langle n-2|\hat{x}|n\rangle$ where, to order λ ,

$$|n\rangle = |n\rangle_0 + \frac{1}{3}m\lambda \sum_{k \neq n} \frac{{}_0\langle k|\hat{x}^3|n\rangle_0}{(n-k)\hbar\omega_0} |k\rangle_0. \quad (71)$$

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 non-zero $O(\lambda)$ amplitude is generated in $\langle n-2|\hat{x}|n\rangle$.

It is straightforward to check that (68) is indeed correct quantum-mechanically; but it is more tedious to check (69), and distinctly unpromising to contemplate checking (70) by doing a conventional perturbation calculation to order $\alpha - 1$. For this particular problem, the ‘improved’ perturbation theory represented by (36) is clearly very useful.

Having calculated the amplitudes for this problem to lowest order, Heisenberg next considers the energy. Unfortunately he again gives no details of his calculation, beyond saying that he uses the classical expression for the energy, namely

$$W = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega_0^2x^2 + \frac{1}{3}m\lambda x^3. \quad (72)$$

It seems a reasonable conjecture, however, that he replaced each term in (72) by its ‘ensemble of representatives’. Thus x^2 , for example, is replaced by the ensemble of terms of the form

$$\sum_{\beta} X(n, n - \beta)X(n - \beta, n - \alpha)e^{i\omega(n, n - \alpha)t}, \quad (73)$$

according to his composition law (10). Similarly, $\dot{x}^2$ is replaced by terms of the form

$$\begin{aligned} & \sum_{\beta} i\omega(n, n - \beta)X(n, n - \beta)e^{i\omega(n, n - \beta)t}i\omega(n - \beta, n - \alpha)X(n - \beta, n - \alpha)e^{i\omega(n - \beta, n - \alpha)t} \\ &= \sum_{\beta} \omega(n, n - \beta)\omega(n - \alpha, n - \beta)X(n, n - \beta)X(n - \beta, n - \alpha)e^{i\omega(n, n - \alpha)t}, \end{aligned} \quad (74)$$

using $\omega(n, m) = -\omega(m, n)$. In general then, in Heisenberg’s scheme, the ‘energy representatives’ will be of the form

$$W(n, n - \alpha)e^{i\omega(n, n - \alpha)t}. \quad (75)$$

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

$$W(n, n - \alpha) = 0, \quad \alpha \neq 0. \quad (76)$$

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 (76) was clearly appreciated by Heisenberg.

To lowest order in λ , the last term in (72) may be dropped. Furthermore, referring to (36), the only λ -independent terms in the X -amplitudes are those involving one-quantum jumps such as $n \rightarrow n - 1$, corresponding in lowest order to amplitudes such as $X^{(0)}(n, n - 1) = \frac{1}{2}a^{(0)}(n, n - 1)$. This means (referring to (73) and (74)) that the elements $W(n, n)$, $W(n, n - 2)$ and $W(n, n + 2)$, and only these $W(n, m)$ ’s, 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 notes), and is given (using (73) and (74) with $\alpha = 0$ and $\beta = \pm 1$) by

$$\begin{aligned}
W(n, n) &= \frac{1}{2}m[\omega^{(0)}(n, n-1)]^2[X^{(0)}(n, n-1)]^2 + \\
&\quad \frac{1}{2}m[\omega^{(0)}(n+1, n)]^2[X^{(0)}(n+1, n)]^2 \\
&\quad + \frac{1}{2}m\omega_0^2[X^{(0)}(n, n-1)]^2 + \frac{1}{2}m\omega_0^2[X^{(0)}(n+1, n)]^2 \\
&= (n + \frac{1}{2})\hbar\omega_0
\end{aligned} \tag{77}$$

using (56), (60) and (61). This is the result given by Heisenberg in H(23).

These ‘lowest order’ results are the only ones Heisenberg reports for the λx^2 force. We do not know whether he carried out higher-order calculations for this case or not. What he writes, next, is that the ‘more precise calculation, taking into account higher order approximations in W, a and 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 only the ‘odd’ terms are present in (36) (i.e. $a_1, \lambda a_3, \lambda^2 a_5$, etc). The results Heisenberg states 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 gives no details of how he has done 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 therefore feel that it is worth giving them here, as being of both pedagogical and historical interest. In the following section we shall obtain the solutions for the λx^2 force (up to order λ^2) which we have been considering hitherto, rather than start afresh with the λx^3 one. The procedure is of course the same for both.

Before leaving the ‘lowest order’ calculations, we address a question which 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 SHO, without going through the apparent device of introducing a perturbation, and then retaining only those parts of the solution which survive as the perturbation vanishes?

For the unperturbed oscillator (the SHO), the equation of motion is of course $\ddot{x} + \omega_0^2 x = 0$, which yields

$$[\omega_0^2 - \omega^2(n, n-\alpha)]X(n, n-\alpha) = 0 \tag{78}$$

for the amplitudes X and frequencies ω . It is also reasonable to retain the ‘quantum condition’ (16), since this is supposed to be true whatever the particular force law. If we *assume* that the only non-vanishing amplitudes are those involving adjacent states (because, for example, in the classical case only a single harmonic is present⁴⁷), then - remembering that $X(n, n-1) = \frac{1}{2}a(n, n-1)$

- (16) and (78) reduce to (57) and (55) respectively, and we quickly recover the previous results. Thus we see that this is indeed an efficient way to solve the quantum SHO⁴⁸. For completeness, however, it would be nice not to have to make the ‘adjacent states’ assumption; Born and Jordan⁴ showed how this could be done, but their argument is somewhat involved. Soon thereafter, of course, the wave-mechanics of Schrödinger, and the operator approach of Dirac, provided the derivations used ever since.

We now turn to the higher order corrections, for the λx^2 force.

3.4 The solutions up to and including λ^2 terms

Consider first equation (51), retaining terms of order λ but no higher powers. We set

$$\omega(n, n-1) = \omega_0 + \lambda\omega^{(1)}(n, n-1) \quad (79)$$

$$a(n, n-1) = a^{(0)}(n, n-1) + \lambda a^{(1)}(n, n-1) \quad (80)$$

and find

$$2\lambda\omega_0\omega^{(1)}(n, n-1)a^{(0)}(n, n-1) = 0, \quad (81)$$

so that

$$\omega^{(1)}(n, n-1) = 0. \quad (82)$$

Consideration of equation (51) up to terms of order λ^2 , employing equations (60), (64) and (68) for the zeroth order amplitudes, gives the $O(\lambda^2)$ correction to $\omega(n, n-1)$ (c.f. (27)):

$$\omega^{(2)}(n, n-1) = -\frac{5\beta^2}{12\omega_0^3}n. \quad (83)$$

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

$$a(n+1, n) = a^{(0)}(n+1, n) + \lambda a^{(1)}(n+1, n) \quad (84)$$

as in (80), and find

$$\sqrt{n+1}a^{(1)}(n+1, n) - \sqrt{n}a^{(1)}(n, n-1) = 0. \quad (85)$$

This equation has the solution $a^{(1)}(n, n-1) = \text{constant}/\sqrt{n}$, but the condition $a^{(1)}(0, -1) = 0$ (c.f. (59)) implies that the constant must be zero, and so

$$a^{(1)}(n, n-1) = 0. \quad (86)$$

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

$$\sqrt{n+1}a^{(2)}(n+1, n) - \sqrt{n}a^{(2)}(n, n-1) = \frac{11\beta^3}{72\omega_0^4}(2n+1), \quad (87)$$

which has the solution

$$a^{(2)}(n, n-1) = \frac{11\beta^3}{72\omega_0^4} n\sqrt{n}. \quad (88)$$

We can now find the higher order corrections to $a(n, n)$ by considering equation (50). We obtain

$$a^{(1)}(n, n) = 0, \quad a^{(2)}(n, n) = -\frac{\beta^4}{72\omega_0^6} (30n^2 + 30n + 11). \quad (89)$$

Similarly, we find from (52)

$$a^{(1)}(n, n-2) = 0, \quad a^{(2)}(n, n-2) = \frac{3\beta^4}{32\omega_0^6} (2n-1)\sqrt{n(n-1)}, \quad (90)$$

where we have used

$$\begin{aligned} \omega^{(2)}(n, n-2) &= \omega^{(2)}(n, n-1) + \omega^{(2)}(n-1, n-2) \\ &= -\frac{5\beta^2}{12\omega_0^3} (2n-1). \end{aligned} \quad (91)$$

These results suffice for our purpose. When n is large, they agree with those obtained for the classical ‘ λx^2 ’ anharmonic oscillator using the method of successive approximations⁴⁹. 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 is given, to order λ^2 , by

$$\begin{aligned} &\frac{1}{2}m\omega_0^2\left\{\frac{1}{4}[(a^{(0)}(n, n-1))^2 + (a^{(0)}(n, n+1))^2] + \frac{\lambda^2}{4}[4(a^{(0)}(n, n))^2 + \right. \\ &2a^{(2)}(n, n-1)a^{(0)}(n-1, n) + 2a^{(2)}(n, n+1)a^{(0)}(n+1, n) + \\ &(a^{(0)}(n, n-2))^2 + (a^{(0)}(n, n+2))^2]\} \\ &= \frac{1}{2}m\omega_0^2\left\{\frac{\beta^2}{2}\left(n + \frac{1}{2}\right) + \frac{5\beta^4\lambda^2}{12\omega_0^4}(n^2 + n + 11/30)\right\}. \end{aligned} \quad (92)$$

Similarly, using (74) up to order λ^2 , with $\alpha = 0$, the (n, n) element of $\frac{1}{2}m\dot{\hat{x}}^2$ is found to be

$$\frac{1}{2}m\omega_0^2\left\{\frac{\beta^2}{2}\left(n + \frac{1}{2}\right) - \frac{5\beta^4\lambda^2}{24\omega_0^4}(n^2 + n + 11/30)\right\}. \quad (93)$$

Finally we need to 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 compute the (n, n) element of $\hat{x}^3$ only to order λ . Using

$$\hat{x}^3(n, n) = \sum_{\alpha} \sum_{\beta} X(n, n-\alpha)X(n-\alpha, n-\beta)X(n-\beta, n) \quad (94)$$

one finds 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). Evaluating these terms using the previously obtained results gives

$$- \frac{5m\lambda^2\beta^4}{24\omega_0^2}(n^2 + n + 11/30) \quad (95)$$

for this term in the energy. Combining (92), (93) and (95) then gives, for the energy up to order λ^2 ,

$$W(n, n) = (n + \frac{1}{2})\hbar\omega_0 - \frac{5\lambda^2\hbar^2}{12m\omega_0^4}(n^2 + n + 11/30), \quad (96)$$

a result⁵⁰ which agrees with classical perturbation theory when n is large⁵¹, and is in exact agreement with standard second-order perturbation theory in quantum mechanics⁵².

As mentioned earlier, Heisenberg does not give results for the ‘ λx^2 ’ force beyond zeroth order; he does, however, give the results for the ‘ λx^3 ’ force 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 operator, which as noted in section 3.3 is independent of time. One should also check that the off-diagonal elements $W(n, n - \alpha)$ vanish (see equation (76)). These are the terms which would (if non-zero) carry a periodic time-dependence, and in his paper Heisenberg says 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 did evaluate, 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 force, up to order λ , as an example of the kind of calculation Heisenberg probably did, finishing it late one night on Heligoland⁵³.

4 Conclusion

We have tried to remove some of the barriers to understanding Heisenberg’s 1925 paper, by providing (apparently for the first time) details of calculations of the type we believe he probably carried out. We hope that more people will thereby be encouraged to appreciate this remarkable paper.

The fact is, Heisenberg’s ‘amplitude calculus’ works: at least for the simple one-dimensional problems on which he tried it out, it is an eminently practical procedure, requiring no sophisticated mathematical knowledge to implement. Since it uses the correct equations of motion, and incorporates the fundamental commutator (11) via the ‘quantum condition’ (16), the answers obtained are completely correct, in the sense of agreeing with conventional quantum mechanics.

We believe that Heisenberg’s approach, as applied to these simple dynamical systems, has considerable pedagogical value, and could usefully be included in

undergraduate courses on quantum mechanics. The multiplication law (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 (10), in formulae such as (22) or the analogous one for the $\lambda\hat{x}^3$ force, introduce the student directly to the fundamental quantum idea that a transition from one state to the other *occurs via all possible intermediate states*, something which can take time to emerge in the traditional wave-mechanical approach. The solution of the quantum SHO, sketched at the end of the previous section, is simple and elementary, 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 of course 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* from Pauli⁵⁴. 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 realisation that the somewhat mysteriously named ‘matrix elements’ of wave-mechanics are indeed the elements of Heisenberg’s matrices.

Appendix A: The quantum condition (16) and $\hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar$.

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

$$\begin{aligned} & \sum_{\alpha} X(n, n - \alpha) i\omega(n - \alpha, n) X(n - \alpha, n) \\ & - \sum_{\alpha} i\omega(n, n - \alpha) X(n, n - \alpha) X(n - \alpha, n). \end{aligned} \quad (97)$$

In the first term of (97), the sum over $\alpha > 0$ may be re-written as

$$-i \sum_{\alpha > 0} \omega(n, n - \alpha) |X(n, n - \alpha)|^2 \quad (98)$$

using $\omega(n, n - \alpha) = -\omega(n - \alpha, n)$ from (1) and $X(n - \alpha, n) = X^*(n, n - \alpha)$ from (45), while the sum over $\alpha < 0$ becomes, similarly,

$$i \sum_{\alpha > 0} \omega(n + \alpha, n) |X(n + \alpha, n)|^2 \quad (99)$$

on changing α to $-\alpha$. Similar steps in the second term of (97) lead to the result

$$\begin{aligned}
(\hat{x}\dot{\hat{x}} - \dot{\hat{x}}\hat{x})(n, n) &= 2i \sum_{\alpha>0} [\omega(n + \alpha, n)|X(n + \alpha, n)|^2 \\
&\quad - \omega(n, n - \alpha)|X(n, n - \alpha)|^2] \\
&= 2i\hbar/(4\pi m),
\end{aligned} \tag{100}$$

where the last step follows from the ‘quantum condition’ (16). Setting $\hat{p} = m\dot{\hat{x}}$ we find

$$(\hat{x}\hat{p} - \hat{p}\hat{x})(n, n) = i\hbar \tag{101}$$

for all values of n . This is the result which Born found³⁶ shortly after reading Heisenberg’s paper. In the further development of the theory the value of the ‘fundamental commutator’ $\hat{x}\hat{p} - \hat{p}\hat{x}$, namely $i\hbar$ times the unit matrix, was taken to be a basic postulate. The sum rule (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 force, up to order λ .

We shall show that, for $\alpha \neq 0$, 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 the qualitative point that, at any given order in λ , only a limited number of elements $W(n, n - 1), W(n, n - 2), \dots$ will contribute, since the amplitudes $X(n, n - \alpha)$ are suppressed by increasing powers of λ as α increases. In fact, for $\alpha \geq 2$ the leading power of λ in $W(n, n - \alpha)$ is $\lambda^{\alpha-2}$, arising 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 only calculate $W(n, n - 1), W(n, n - 2), W(n, n - 3)$.

(a) $W(n, n - 1)$

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

$$\begin{aligned}
&\frac{1}{4}m\omega_0^2\lambda\{a^{(0)}(n, n)a^{(0)}(n, n - 1) + a^{(0)}(n, n - 1)a^{(0)}(n - 1, n - 1) + \\
&\frac{1}{2}[a^{(0)}(n, n + 1)a^{(0)}(n + 1, n - 1) + a^{(0)}(n, n - 2)a^{(0)}(n - 2, n - 1)]\} \\
&= -\frac{5}{24}m\lambda\beta^3n\sqrt{n}.
\end{aligned} \tag{102}$$

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

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

$$\begin{aligned}
& \omega^{(0)}(n, n-2)\omega^{(0)}(n-2, n-1)a^{(0)}(n, n-2)a^{(0)}(n-2, n-1)\} \\
& = \frac{1}{12}m\lambda\beta^3 n\sqrt{n}.
\end{aligned} \tag{103}$$

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

$$\begin{aligned}
& \frac{1}{24}m\lambda\{a^{(0)}(n, n-1)a^{(0)}(n-1, n)a^{(0)}(n, n-1) + \\
& a^{(0)}(n, n-1)a^{(0)}(n-1, n-2)a^{(0)}(n-2, n-1) \\
& + a^{(0)}(n, n+1)a^{(0)}(n+1, n)a^{(0)}(n, n-1)\} \\
& = \frac{1}{8}m\lambda\beta^3 n\sqrt{n}.
\end{aligned} \tag{104}$$

The sum of (102), (103) and (104) 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

$$\frac{1}{8}m\omega_0^2 a^{(0)}(n, n-1)a^{(0)}(n-1, n-2), \tag{105}$$

which is cancelled 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 $\frac{1}{2}m\omega_0^2\hat{x}^2$:

$$\begin{aligned}
& \frac{1}{8}m\omega_0^2\lambda\{a^{(0)}(n, n-1)a^{(0)}(n-1, n-3) + a^{(0)}(n, n-2)a^{(0)}(n-2, n-3)\} \\
& = \frac{1}{24}m\lambda\beta^3\sqrt{n(n-1)(n-2)}.
\end{aligned} \tag{106}$$

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

$$\begin{aligned}
& -\frac{1}{8}m\lambda\{\omega^{(0)}(n, n-1)a^{(0)}(n, n-1)\omega^{(0)}(n-1, n-3)a^{(0)}(n-1, n-3) \\
& + \omega^{(0)}(n, n-2)a^{(0)}(n, n-2)\omega^{(0)}(n-2, n-3)a^{(0)}(n-2, n-3)\}
\end{aligned} \tag{107}$$

$$= -\frac{1}{12}\lambda m\beta^3\sqrt{n(n-1)(n-2)}. \tag{108}$$

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

$$\begin{aligned}
& \frac{1}{24}m\lambda a^{(0)}(n, n-1)a^{(0)}(n-1, n-2)a^{(0)}(n-2, n-3) \\
& = \frac{1}{24}\lambda m\beta^3\sqrt{n(n-1)(n-2)}.
\end{aligned} \tag{109}$$

The sum of (106), (108) and (109) vanishes, as required.

- 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 of the paper which is included as paper 12 in Ref. 3, pp. 261-276. In the present paper we shall refer exclusively to this translation; in particular, we shall refer to the equations in it as ‘H(1), H(2) . . . ’ etc.
- ³ *Sources of Quantum Mechanics*, edited by B. L. van der Waerden (Amsterdam, North-Holland, 1967).
- ⁴ M. Born and P. Jordan, “Zur Quantenmechanik”, Z. Phys. **34**, 858-888 (1925), reprinted in translation as paper 13 in Ref. 3.
- ⁵ P. A. M. Dirac, “The Fundamental Equations of Quantum Mechanics”, Proc. Roy. Soc. 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), reprinted in translation as paper 15 in Ref. 3.
- ⁷ S. Weinberg, *Dreams of a Final Theory* (New York, Pantheon, 1992).
- ⁸ S.-I. Tomonaga, *Quantum Mechanics Volume 1 Old Quantum Theory* (Amsterdam, North-Holland, 1962).
- ⁹ M. Jammer, *The Conceptual Development of Quantum Mechanics* (New York, McGraw-Hill, 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* vol 2 (New York, Springer-Verlag, 1982).
- ¹² J. Hendry, *The Creation of Quantum Mechanics and the Bohr-Pauli Dialogue* (Dordrecht, D. Reidel, 1984).
- ¹³ T.-Y. Wu, *Quantum Mechanics* (Singapore, World Scientific, 1986).
- ¹⁴ M. Taketani and M. Nagasaki, *The Formation and Logic of Quantum Mechanics* vol 3 (Singapore, World Scientific, 2002).
- ¹⁵ G. Birtwistle, *The New Quantum Mechanics* (Cambridge, Cambridge University Press, 1928).
- ¹⁶ M. Born, *Atomic Physics* (New York, Dover, 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* vol 2 (Singapore, World Scientific, 2001).
- ¹⁹ Ref. 7, page 53.
- ²⁰ All quotations are from the English translation in Ref. 3.
- ²¹ We use ω here rather than Heisenberg’s ν .
- ²² The reader may find it helpful at this point to consult Ref. 23, 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* 2nd edtn (New York, Wiley, 1975), section 9.2.
- ²³ W. A. Fedak and J. J. Prentis, “Quantum jumps and classical harmonics”, Am. J. Phys. **70**, 332-344 (2002).
- ²⁴ We depart from the Gothic notation of Ref. 3 (and Ref. 1), preferring

that of Tomonaga, Ref. 8, pp 204-224. 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 $X_{-|\alpha|}(n)\exp[-i\omega(n)|\alpha|t]$. Replacing $-\omega(n)|\alpha|$ by $-\omega(n, n - |\alpha|)$, which is equal to $\omega(n - |\alpha|, n)$ using (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 since $\omega(n, n + |\alpha|)$ is not the same, in general, as $\omega(n - |\alpha|, n)$.

²⁵ 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, for ease of reference.

²⁶ This step apparently did not occur to him immediately - see Ref. 11, page 231.

²⁷ 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 writes before H(20).

²⁸ W. Thomas, "Über die Zahl der Dispersionelektronen, die einem stationären Zustande zugeordnet sind (Vorläufige Mitteilung)", *Naturwiss.* **13**, 627 (1925).

²⁹ W. Kuhn, "Über die Gesamtstärke der von einem Zustande ausgehenden Absorptionslinien", *Z. Phys.* **33** 408-412(1925), reprinted in translation as paper 11 in ref. 3.

³⁰ W. Heisenberg, as discussed in Ref. 11 pages 243 ff.

³¹ Ref. 9, p 193; Φ is any function defined for stationary states.

³² M. Born, "Über Quantenmechanik", *Z. Phys.* **26**, 379-395 (1924), reprinted in translation as paper 7 in ref. 3.

³³ Ref. 9, p 202.

³⁴ H. A. Kramers and W. Heisenberg, "Über die Streuung von Strahlen durch Atome", *Z. Phys.* **31**, 681-707 (1925), reprinted in translation as paper 10 in Ref. 3.

³⁵ For considerable further detail on dispersion theory, sum rules, and the 'discretisation' rules see Ref. 8 pages 142-147 and pages 206-208, and Ref. 9 section 4.3.

³⁶ See Ref. 3 page 37.

³⁷ For an interesting discussion of the possible reasons why he chose to try out his scheme on the anharmonic oscillator, see Ref. 11 pages 232-235; and also Ref. 3 page 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.

³⁸ The $(n, n - \alpha)$ matrix element, in the standard terminology.

³⁹ Equation (22) is not in Heisenberg's paper, though it is given by Tomonaga, Ref. 8, equation (32.20').

⁴⁰ Note that this means that, in $x(t)$, 'all the terms which are of order λ^p ' arise from many different terms in (24).

⁴¹ Except that Heisenberg re-labels most of the a_α 's as $a_\alpha(n)$.

⁴² Actually he writes $a_0(n)$ in place of $a(n, n)$ in (40), through an oversight.

⁴³ MacKinnon (Ref. 10) suggests how, in terms of concepts from the 'virtual oscillator' model, equations (32) - (35) may be 'transformed' into equations (40) - (43); we do not agree with MacKinnon (Ref. 10, footnote 62) regarding 'mis-

takes' in (42) and (43).

⁴⁴ In the version of the quantum condition which Heisenberg gives just before H(20), he unfortunately uses the same symbol for the transition amplitudes as in H(16) - see our (16) - but replaces ' $4\pi m$ ' by ' πm ', not explaining where the factor $1/4$ has come from (see (49)); he also omits the λ 's.

⁴⁵ Heisenberg omits the superscripts.

⁴⁶ See for example L. I. Schiff, *Quantum Mechanics*, 3rd edtn New York, McGraw-Hill, 1968).

⁴⁷ This is the justification suggested by Born and Jordan in Ref. 4.

⁴⁸ It is essentially that given by L. D. Landau and E. M. Lifshitz, *Course of Theoretical Physics Vol. 3 Quantum Mechanics* 3rd edtn (Oxford, Pergamon, 1977), pages 67-68.

⁴⁹ L. D. Landau and E. M. Lifshitz, *Course of Theoretical Physics Vol. 1 Mechanics* 3rd edtn (Oxford, Pergamon, 1976).

⁵⁰ This equation corresponds to equation (88) of Born and Jordan's paper, Ref. 4, in which there appears to be a misprint of $17/30$ for $11/30$.

⁵¹ See Ref. 4.

⁵² L. D. Landau and E. M. Lifshitz, as cited in Ref. 48, page 136.

⁵³ See W. Heisenberg, *Physics and Beyond* (London, Allen & Unwin, 1971), page 61.

⁵⁴ W. Pauli, "Über das Wasserstoffspektrum vom Standpunkt der neuen Quantenmechanik", Z. Phys. **36**, 336-363 (1926), reprinted in translation as paper 16 in Ref. 3.