Chapter 1

Introduction

1.1 Origin and Discovery of Quantum Mechanics

The observation made by Planck towards the end of 1900, that the formula he had established for the energy distribution of electromagnetic black body radiation was in agreement with the experimentally confirmed Wien- and Rayleigh–Jeans laws for the limiting cases of small and large values of the wave-length λ (or λT) respectively is generally considered as the discovery of quantum mechanics. Planck had arrived at his formula with the assumption of a distribution of a countable number of infinitely many oscillators. We do not enter here into detailed considerations of Planck, which involved also thermodynamics and statistical mechanics (in the sense of Boltzmann's statistical interpretation of entropy). Instead, we want to single out the vital aspect which can be considered as the discovery of quantum mechanics. Although practically every book on quantum mechanics refers at the beginning to Planck's discovery, very few explain in this context what he really did in view of involvement with statistical mechanics.

A "perfectly black body" is defined to be one that absorbs all (thermal) radiation incident on it. The best approximation to such a body is a cavity with a tiny opening (of solid angle $d\Omega$) and whose inside walls provide a diffuse distribution of the radiation entering through the hole with the intensity of the incoming ray decreasing rapidly after a few reflections from the walls. Thermal radiation (with wave-lengths $\lambda \sim 10^{-5}$ to 10^{-2} cm at moderate temperatures T) is the radiation emitted by a body (consisting of a large number of atoms) as a result of the temperature (as we know today as a result of transitions between a large number of very closely lying energy levels). Kirchhoff's law in thermodynamics says that in the case of equilibrium, the amount of radiation absorbed by a body is equal to the amount the body emits. Black bodies as good absorbers are therefore also good emitters, i.e. radiators. The (equilibrium) radiation of the black body can be determined experimentally by sending radiation into a cavity surrounded by a heat bath at temperature T, and then measuring the increase in temperature of the heat bath.

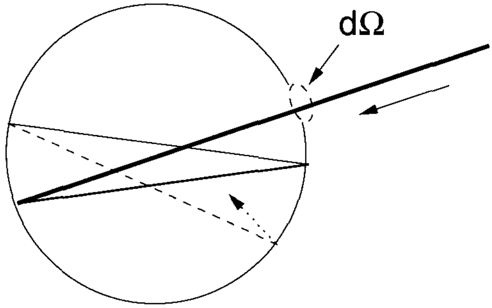

Fig. 1.1 Absorption in a cavity.

Let us look at the final result of Planck, i.e. the formula (to be explained)

$$\bar{u}(\nu, T) = 2\frac{4\pi\nu^2}{c^3}\left(\frac{x}{e^x - 1}\right)kT, \quad \text{where } x = \frac{h\nu}{kT} = \frac{hc}{k\lambda T}. \tag{1.1}$$

Here $\bar{u}(\nu, T)d\nu$ is the mean energy density (i.e. energy per unit volume) of the radiation (i.e. of the photons or photon gas) in the cavity with both possible directions of polarization (hence the factor "2") in the frequency domain $\nu, \nu + d\nu$ in equilibrium with the black body at temperature T. In Eq. (1.1) c is the velocity of light with $c = \nu\lambda, \lambda$ being the wave-length of the radiation. The parameters k and h are the constants of Boltzmann and Planck:

$$k = 1.38 \times 10^{-23} J\, K^{-1}, \quad h = 6.626 \times 10^{-34} J\, s.$$

How did Planck arrive at the expression (1.1) containing the constant h by treating the radiation in the cavity as something like a gas? By 1900 two theoretically-motivated (but from today's point of view incorrectly derived) expressions for $\bar{u}(\nu, T)$ were known and tested experimentally. It was found that one expression agreed well with observations in the region of small λ (or λT), and the other in the region of large λ (or λT). These expressions are:
(1) *Wien's law*:

$$\bar{u}(\nu, T) = C_1\nu^3 e^{-C_2\nu/T}, \tag{1.2}$$

and the

(2) *Rayleigh–Jeans law*:

$$\bar{u}(\nu, T) = 2\frac{4\pi\nu^2}{c^3}C_3T, \tag{1.3}$$

C_i, C_2, C_3 being constants.
Considering Eq. (1.1) in regions of x "small" (i.e. $\exp(x) \simeq 1+x$) and "large" ($\exp(-x) \ll 1$), we obtain:

$$\begin{aligned} \bar{u}(\nu, T) &\simeq 2\frac{4\pi\nu^2}{c^3}kT, \quad (x \text{ small}), \\ \bar{u}(\nu, T) &\simeq 2\frac{4\pi\nu^2}{c^3}e^{-x}h\nu, \quad (x \text{ large}). \end{aligned}$$

We see, that the formulas (1.2) and (1.3) are contained in Eq. (1.1) as approximations. Indeed, in the first place Planck had tried to find an expression linking both, and he had succeeded in finding such an expression of the form

$$\bar{u}(\nu, T) = \frac{a\nu^3}{e^{b\nu/T} - 1},$$

where a and b are constants. When Planck had found this expression, he searched for a derivation. To this end he considered Boltzmann's formula $S = k \ln W$ for the entropy S. Here W is a number which determines the distribution of the energy among a discrete number of objects, and thus over a discrete number of admissible states. This is the point, where the

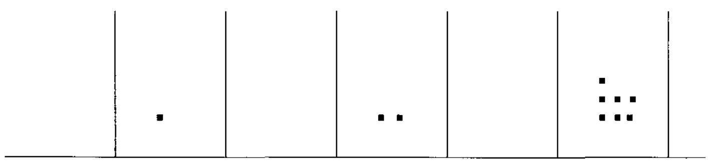

Fig. 1.2 Distributing quanta (dots) among oscillators (boxes).

discretization begins to enter. Planck now imagined a number N of oscillators or N oscillating degrees of freedom, every oscillator corresponding to an eigenmode or eigenvibration or standing wave in the cavity and with mean energy U. Moreover Planck assumed that these oscillators do not absorb or emit energy continuously, but — here the discreteness appears properly — only in elements (quanta) ϵ, so that W represents the number of possible ways of distributing the number $P := NU/\epsilon$ of energy-quanta ("photons", which are indistinguishable) among the N indistinguishable oscillators at temperature T, $U(T)$ being the average energy emitted by one oscillator. We visualize the N oscillators as boxes separated by $N-1$ walls, with the quanta represented schematically by dots as indicated in Fig. 1.2. Then W is given by

$$W = \frac{(N+P-1)!}{(N-1)!P!}. \tag{1.4}$$

With the help of *Stirling's formula**

$$\ln N! \simeq N \ln N - N + O(0), \quad N \to \infty,$$

and the second law of thermodynamics $((\partial S/\partial U)_V = 1/T)$, one obtains (cf. Example 1.1)

$$U = \frac{\epsilon}{e^{\epsilon/kT} - 1} \tag{1.5}$$

as the mean energy emitted or absorbed by an oscillator (corresponding to the classical expression of $2 \times kT/2$, as for small values of ϵ). Agreement with Eq. (1.2) requires that $\epsilon \propto \nu$, i.e.

$$\epsilon = h\nu, \quad h = \text{const.} \tag{1.6}$$

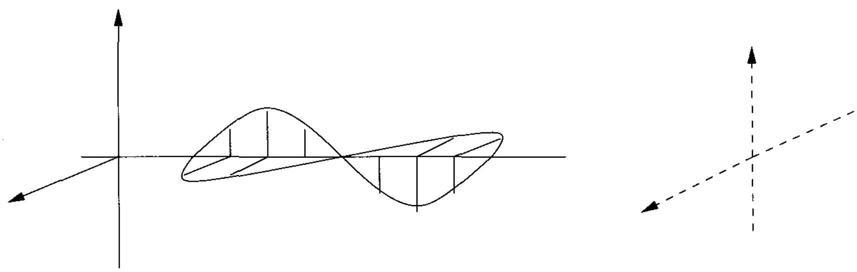

Fig. 1.3 Comparing the polarization modes with those of a 2-dimensional oscillator.

We now obtain the energy density of the radiation, $\bar{u}(\nu, T)d\nu$, by multiplying U with the number $n_\nu d\nu$ of modes or oscillators per unit volume with frequency ν in the interval $\nu, \nu + d\nu$, i.e. with

$$n_\nu d\nu = 2 \times \frac{4\pi\nu^2}{c^3} d\nu, \tag{1.7}$$

*See e.g. I. S. Gradshteyn and I. M. Ryzhik [122], formula 8.343(2), p. 940, there not called Stirling's formula, as in most other Tables, e.g. W. Magnus and F. Oberhettinger [181], p.3. The Stirling formula or approximation will appear frequently in later chapters.

where the factor 2 takes the two possible mutually orthogonal linear directions of polarization of the electromagnetic radiation into account, as indicated in Fig.1.3. We obtain the expression (1.7) for instance, as in electrodynamics, where we have for the electric field

$$\mathbf{E} \propto e^{i\omega t} \sum_{\boldsymbol{\kappa}} \mathbf{e}_{\boldsymbol{\kappa}} \sin \kappa_1 x_1 \sin \kappa_2 x_2 \sin \kappa_3 x_3$$

with the boundary condition that at the walls $\mathbf{E} = 0$ at $x_i = 0, L$ for $i = 1, 2, 3$ (as for ideal conductors). Then $L\kappa_i = \pi n_i$, $n_i = 1, 2, 3, \ldots$,

$$L^2 \boldsymbol{\kappa}^2 = \pi^2 \mathbf{n}^2,$$

where†

$$\boldsymbol{\kappa}^2 = \left(\frac{2\pi\nu}{c}\right)^2, \quad \text{so that} \quad \left(\frac{2\nu L}{c}\right)^2 = \mathbf{n}^2.$$

The number of possible modes (states) is equal to the volume of the spherical octant (where $n_i > 0$) in the space of $n_i, i = 1, 2, 3$. The number with frequency ν in the interval $\nu, \nu + d\nu$, i.e. $n_\nu d\nu$ per unit volume, is given by

$$\begin{aligned} d\mathcal{N} &= \frac{d\mathcal{N}}{d\nu} d\nu \equiv n_\nu d\nu = \frac{d}{d\nu}\left[\frac{1}{8}\frac{4}{3}\pi\left(\frac{2\nu L}{c}\right)^3 / L^3\right] d\nu \\ &= \frac{1}{8}\frac{4}{3}\pi\frac{8}{c^3} 3\nu^2 d\nu = \frac{4\pi\nu^2}{c^3} d\nu, \end{aligned}$$

as claimed in Eq. (1.7). We obtain therefore

$$\bar{u}(\nu, T) = U n_\nu = 2\frac{4\pi\nu^2}{c^3}\frac{h\nu}{e^{h\nu/kT} - 1}. \tag{1.8}$$

This is *Planck's formula* (1.1). We observe that $\bar{u}(\nu, T)$ has a maximum which follows from $d\bar{u}/d\lambda = 0$ (with $c = \nu\lambda$). In terms of λ we have

$$\bar{u}(\lambda, T) d\lambda = \frac{8\pi}{\lambda^4}\frac{hc/\lambda}{e^{hc/\lambda kT} - 1} d\lambda,$$

so that the derivative of $\bar{u}$ implies (x as in Eq. (1.1))

$$\left(1 - \frac{x}{5}\right) e^x = 1.$$

The solutions of this equation are

$$x_{\text{max}} = 4.965 \quad \text{and} \quad x_{\text{min}} = 0.$$

† From the equation $\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \boldsymbol{\nabla}^2\right)\mathbf{E} = 0$, so that $-\omega^2/c^2 + \boldsymbol{\kappa}^2 = 0, \omega = 2\pi\nu$.

The first value yields

$$\lambda_{\max}T = \frac{hc}{4.965k} = \text{const.}$$

This is Wien's *displacement law*, which had also been known before Planck's discovery, and from which the constant h *can be determined* from the known value of k.

Later it was realized by H. A. Lorentz and Planck that Eq. (1.8) could be derived much more easily in the context of statistical mechanics. If an oscillator with thermal weight or occupation probability $\exp(-nx)$ can assume only discrete energies $\epsilon_n = nh\nu$, $n = 0, 1, 2, \ldots$, then (with $x = h\nu/kT$) its mean energy is

$$\begin{aligned} U &= \frac{\sum_{n=0}^{\infty} nh\nu e^{-nx}}{\sum_{n=0}^{\infty} e^{-nx}} = -h\nu\frac{d}{dx}\ln\sum_{n=0}^{\infty} e^{-nx} \\ &= -h\nu\frac{d}{dx}\ln\frac{1}{1-e^{-x}} = h\nu\frac{(1-e^{-x})}{(1-e^{-x})^2}e^{-x} \\ &= \frac{h\nu}{e^x - 1}. \end{aligned} \quad (1.9)$$

We observe that for $T \to 0$ (i.e. $x \to \infty$) the mean energy vanishes ($0 < U \leq \infty$). Thus we have a rather complicated system here, that of an oscillation system at absolute temperature $T \neq 0$. One expects, of course, that it is easier to consider first the case of $T = 0$, i.e. the behaviour of the system at zero absolute temperature. Since temperature originates through contact with other oscillators, we then have at $T = 0$ independent oscillators, which can assume the discrete energies $\epsilon_n = nh\nu$. We are not dealing with the linear harmonic oscillator familiar from mechanics here, but one can expect an analogy. We shall see later that in the case of this *linear harmonic oscillator* the energies E_n are given by

$$E_n = \left(n + \frac{1}{2}\right)h\nu \equiv \left(n + \frac{1}{2}\right)\hbar\omega, \quad \hbar = \frac{h}{2\pi}, \quad n = 0, 1, 2. \ldots. \quad (1.10)$$

Thus here the so-called *zero point energy* appears, which did not arise in Planck's consideration of 1900.

One might suppose now, that we arrive at quantum mechanics simply by discretizing the energy and thus by postulating — following Planck — for the harmonic oscillator the expression (1.10). However, such a procedure leads to contradictions, which can not be eliminated without a different approach. We therefore examine such contradictions next.

Example 1.1: Mean energy of an oscillator

In Boltzmann's statistical mechanics the entropy S is given by the following expression (which we cite here with no further explanation) $S = k \ln W$, where k is Boltzmann's constant and W is the number of times P indistinguishable elements of energy ϵ can be distributed among N indistinguishable oscillators, i.e.

$$W = \frac{(N+P-1)!}{(N-1)!P!}, \quad \text{and} \quad P = \frac{UN}{\epsilon}.$$

Show with the help of Stirling's formula that the mean energy U of an oscillator is given by

$$U = \frac{\epsilon}{\exp(\epsilon/kT) - 1}.$$

Solution: Inserting W into Boltzmann's formula and using $\ln N! \simeq N \ln N - N$, we obtain

$$S = k[\ln(N+P-1)! - \ln(N-1)! - \ln P!] \simeq kN\left[\left(1+\frac{U}{\epsilon}\right)\ln\left(1+\frac{U}{\epsilon}\right) - \frac{U}{\epsilon}\ln\frac{U}{\epsilon}\right].$$

The second law of thermodynamics says

$$\left(\frac{\partial S}{\partial U}\right)_V = \frac{1}{T}.$$

For a single oscillator the entropy is $s = S/N$, so that

$$\frac{1}{T} = \left(\frac{\partial s}{\partial U}\right)_V = k\frac{\partial}{\partial U}\left[\left(1+\frac{U}{\epsilon}\right)\ln\left(1+\frac{U}{\epsilon}\right) - \frac{U}{\epsilon}\ln\frac{U}{\epsilon}\right] = \frac{k}{\epsilon}\ln\left(\frac{\epsilon}{U}+1\right),$$

i.e.

$$U = \frac{\epsilon}{\exp(\epsilon/kT) - 1},$$

which for $\epsilon/kT \to 0$ becomes

$$U \simeq \frac{\epsilon}{1 + \frac{\epsilon}{kT} - 1} \simeq kT.$$

This means U is then the classical expression resulting from the mean kinetic energy per degree of freedom, $kT/2$, for 2 degrees of freedom.

1.2 Contradicting Discretization: Uncertainties

The far-reaching consequences of Planck's quantization hypothesis were recognized only later, around 1926, with Heisenberg's discovery of the uncertainty relation. In the following we attempt to incorporate the above discretizations into classical considerations* and consider for this reason so-called *thought experiments* (from German "Gedankenexperimente"). We

*This is what was effectively done before 1925 in Bohr's and Sommerfeld's atomic models and is today referred to as "*old quantum theory*".

shall see that we arrive at contradictions. As an example[†] we consider the *linear harmonic oscillator* with energy

$$E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2 x^2. \tag{1.11}$$

The classical equation of motion

$$\frac{dE}{dt} = \dot{x}(m\ddot{x} + m\omega^2 x) = 0$$

permits solutions $x = A\cos(\omega t + \delta)$, so that

$$E = \frac{1}{2}m\omega^2 A^2,$$

where A is the maximum displacement of the oscillation, i.e. at $\dot{x} = 0$. We consider first this case of velocity and hence momentum precisely zero, and investigate the possibility to fix the amplitude. If we replace E by the discretized expression (1.10), i.e. by $E_n = (n + 1/2)\hbar\omega$, we obtain for the amplitude A

$$A \longrightarrow A_n = \sqrt{\frac{2\hbar}{m\omega}}\sqrt{n + \frac{1}{2}}. \tag{1.12}$$

Thus the amplitude can assume only these definite values. We now perform the following thought experiment. We give the oscillator initially an amplitude which is not contained in the set (1.12), i.e. for instance an amplitude $\tilde{A}$ with

$$A_n < \tilde{A} < A_{n+1}.$$

Energy conservation then requires that the oscillator has to oscillate all the time with this (according to Eq. (1.12) nonpermissible) amplitude. In order to be able to perform this experiment, the difference

$$\triangle A = A_{n+1} - A_n$$

must not be too small, i.e. the difference

$$\triangle A = \sqrt{\frac{2\hbar}{m\omega}}\left(\sqrt{n + \frac{3}{2}} - \sqrt{n + \frac{1}{2}}\right) \simeq \sqrt{\frac{2\hbar}{m\omega}}\frac{2}{4\sqrt{n}}[1 + O(1/n)].$$

For $m = 2kg$, $\hbar = 1 \times 10^{-34} J\,s$, $\omega = 1s^{-1}$, we obtain

$$\triangle A \simeq \frac{10^{-17}}{2\sqrt{n}}[1 + O(1/n)] \quad \text{meter}.$$

[†]H. Koppe [152].

This distance is even less than what one would consider as a certain "diameter" of the electron ($\sim 10^{-15}$ meter). Thus it is even experimentally impossible to fix the amplitude $\tilde{A}$ of the oscillator with the required precision. Since A is the largest value of x, where $\dot{x} = 0$, we have the problem that for a given definite value of $m\dot{x}$, i.e. zero, the value of $x = A$ can not be determined, i.e. given the energy of Eq. (1.10), it is *not possible* to give the oscillator at the same time at a definite position a definite momentum.

The above expression (1.10) for the energy of the harmonic oscillator, which we have not established so far, has the further characteristic of possessing the "*zero-point energy*" $\hbar\omega/2$, the smallest energy the oscillator can assume, according to the formula. Let us now consider the oscillator as a pendulum with frequency ω in the gravitational field of the Earth.[‡] Then

$$\omega^2 = \frac{g}{l}, \tag{1.13}$$

where l is the length of the pendulum. Thus we can vary the frequency ω by varying the length l. This can be achieved with the help of a pivot, attached to a movable frame as indicated in Fig. 1.4. The resultant of the tension in the string of the pendulum, $\mathbf{R}$, always has a nonnegative vertical component. If the pivot is moved downward, work is done against this vertical component of $\mathbf{R}$; in other words, the system receives additional energy. However, there is one case, in which for a very short interval of time, δt, the pendulum is at angle $\theta = 0$. Reducing in this short interval of time the length of the pendulum (by an appropriately quick shift of the pivot) by a factor of 4, the frequency of the oscillator is doubled, without supplying it with additional energy. Thus the energy

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad \text{becomes} \quad \left(n + \frac{1}{2}\right)\hbar\, 2\omega,$$

without giving it additional energy. This is a self-evident *contradiction*. This means — if the quantum mechanical expression (1.10) is valid — we cannot simultaneously fix the energy (with energy conservation), as well as time t to an interval $\delta t \to 0$.[§]

The source of our difficulties in the considerations of these two examples is that in both cases we try to incorporate the discrete energies (1.10) into the framework of classical mechanics without any changes in the latter. Thus the theory with discrete energies must be very different from classical mechanics with its continuously variable energies.

[‡] H. Koppe [152].

[§] See also Example 1.3.

It is illuminating in this context to consider the linear oscillator in phase space (q, p) with

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 = \text{const.} \tag{1.14}$$

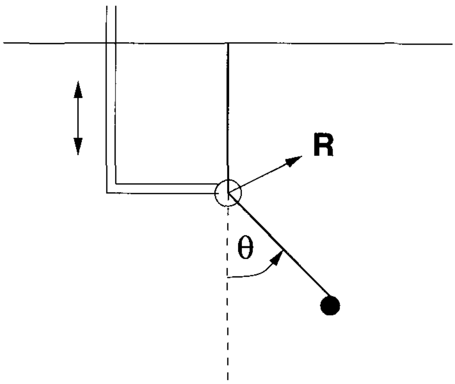

Fig. 1.4 The pendulum with variable length.

This equation is that of an ellipse as a comparison with the Cartesian form

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$$

reveals immediately. Evidently the ellipses in the (q, p)-plane have semi-axes of lengths

$$a = \sqrt{\frac{2E}{m\omega^2}}, \qquad b = \sqrt{2mE}. \tag{1.15}$$

Inserting here (1.10), we obtain

$$a_n = \sqrt{\frac{2(n+1/2)\hbar\omega}{m\omega^2}}, \qquad b_n = \sqrt{2m(n+1/2)\hbar\omega}. \tag{1.16}$$

We see that for $n = 0, 1, 2, \ldots$ only certain ellipses are allowed. The area enclosed by such an ellipse is (note A earlier amplitude, now means area)

$$A_n = \pi a_n b_n = \frac{2\pi E_n}{\omega} = 2\pi\hbar\left(n + \frac{1}{2}\right), \tag{1.17a}$$

or

$$\oint p\,dq = 2\pi\hbar\left(n + \frac{1}{2}\right). \tag{1.17b}$$

In the first of the examples discussed above the contradiction arose as a consequence of our assumption that we could put the oscillator initially at any point in phase space, i.e. at some point which does not belong to one of the allowed ellipses. In the second example we chose $n = 0$ and thus restricted ourselves to the innermost orbit. However, we also assumed we would know at which point of the orbit the pendulum could be found.

Thus in attempting to incorporate the discrete quantization condition into the context of classical mechanics we see, that a system cannot be localized with arbitrary precision in phase space, in other words the area $\triangle A$, in which a system can be localized, is not nought. We can write this area

$$\triangle A \geq A_{n+1} - A_n \stackrel{(1.17a)}{=} 2\pi\hbar,$$

since the system cannot be "between" A_{n+1} and A_n. Since $\triangle A$ represents an element of area of the (q,p)-plane, we can write more precisely

$$\triangle p \triangle q \geq 2\pi\hbar. \tag{1.18}$$

This relation, called the *Heisenberg uncertainty relation*, implies that if we wish to make q very precise by arranging $\triangle q$ to be very small, the complementary uncertainty in momentum, $\triangle p$, becomes correspondingly large and extends over a large number of quantum states, as — for instance — in the second example considered above and illustrated in Fig. 1.5.

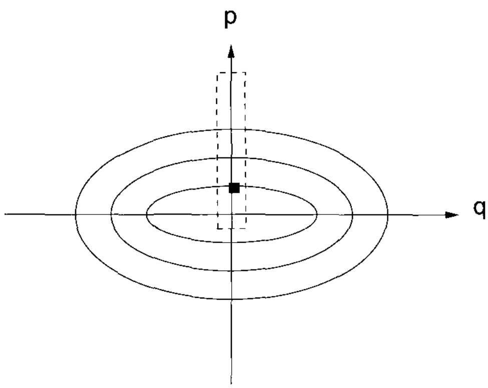

Fig. 1.5 Precise q implying large uncertainty in p.

Thus we face the problem of formulating classical mechanics in such a way that by some kind of extension or generalization we can find a way to quantum mechanics. Instead of the deterministic Newtonian mechanics — which for a given precise initial position and initial momentum of a system yields the precise values of these for any later time — we require a formulation answering the question: If the system is at time $t = 0$ in the area defined by the limits

$$0 \leq q \leq q + \Delta q, \quad 0 \leq p \leq p + \Delta p,$$

what can be said about its position at some later time $t = T$? The appropriate formulation does not yet have anything to do with quantum mechanics; however, it permits the transition to quantum mechanics, as we shall see. Before we continue in this direction, we return once again briefly to the historical development, and there to the ideas leading to *particle-wave duality.*¶

1.3 Particle-Wave Dualism

The wave nature of light can be deduced from the phenomenon of interference, as in a double-slit experiment, as illustrated in Fig. 1.6.

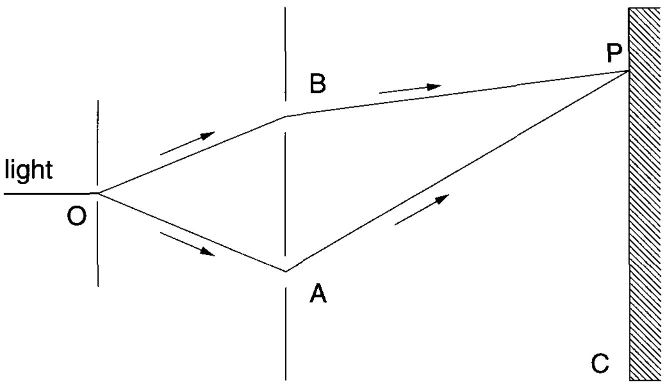

Fig. 1.6 Schematic arrangement of the double-slit experiment.

Light of wave-length λ from a source point O can reach point P on the observation screen C either through slit A or through slit B in the diaphragm placed somewhere in between. If the difference of the path lengths OBP, OAP is $n\lambda, n \in \mathbb{Z}$, the wave at P is re-inforced by superposition and one observes a bright spot; if the difference is $n\lambda/2$, the waves annul each other and one observes a dark spot. Both observations can be understood by a wave propagation of light. The *photoelectric effect*, however, seems to suggest a corpuscular nature of light. In this effect* light of frequency ν is sent onto a metal plate in a vacuum, and the electrons ejected by the light from the plate are observed by applying a potential difference between this plate and another one. The energy of the observed electrons depends only on ν and

¶See also M.–C. Combourieu and H. Rauch [58].

*This is explained in experimental physics; we therefore do not enter into a deeper explanation here.

the number of such *photo-electrons* on the intensity of the incoming light. This is true even for very weak light. Einstein concluded from this effect, that the energy in a light ray is transported in the form of localized packets, called *wave packets*, which are also described as *photons* or *quanta.* Indeed the Compton effect, i.e. the elastic scattering of light, demonstrates that photons can be scattered off electrons like particles. Thus whereas Planck postulated that an oscillator emits or absorbs radiation in units of $h\nu = \hbar\omega$, Einstein went further and postulated that radiation consists of discrete quanta.

Thus light can be attributed a wave nature but also a corpuscular, i.e. particle-like, nature. In the interference experiment light behaves like a wave, but in the photoelectric effect like a stream of particles. One could try to play a trick, and use radiation which is so weak that it can transport only very few photons. What does the interference pattern then look like? Instead of bands one observes a few point-like spots. With an increasing number of photons these spots become denser and produce bands. Thus the interference experiment is always indicative of the wave nature of light, whereas the photoelectric effect is indicative of its particle-like nature. Without going into further historical details we add here, that it was Einstein in 1905 who attributed a momentum p to the light quantum with energy $E = h\nu$, and both he and Planck attributed to this the momentum

$$p = \frac{h\nu}{c} = \frac{h}{\lambda}. \tag{1.19}$$

The hypothesis that every freely moving nonrelativistic microscopic particle with energy E and momentum $\mathbf{p}$ can be attributed a plane harmonic matter wave $\psi(\mathbf{r}, t)$ was put forward much later, i.e. in 1924, by de Broglie.† This wave can be written as a complex function

$$\psi(\mathbf{r}, t) = Ae^{i\mathbf{k}\cdot\mathbf{r}-i\omega t},$$

where $\mathbf{r}$ is the position vector, and ω and $\mathbf{k}$ are given by

$$E = \hbar\omega, \quad \mathbf{p} = \hbar\mathbf{k}.$$

Thus particles also possess a wave-like nature. It is wellknown that this was experimentally verified by Davisson and Germer [64], who demonstrated the existence of electron waves by the observation of diffraction fringes instead of intensity distributions in appropriate experiments.

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†L. de Broglie [39].

1.4 Particle-Wave Dualism and Uncertainties

We saw above that we can observe the wave nature of light in one type of experiment, and its particle-like nature in another. We cannot observe both types simultaneously, i.e. the wave-like nature together with the particle-like nature. Thus these wave and particle aspects are complementary, and show up only under specific experimental situations. In fact, they exclude each other. Every attempt to single out either of these aspects, requires a modification of the experiment which rules out every possibility to observe the other aspect.‡ This becomes particularly clear, if in a double-slit experiment the detectors which register outcoming photons are placed immediately behind the diaphragm with the two slits: A photon is registered only in one detector, not in both — hence it cannot split itself. Applying the above uncertainty principle to this situation, we identify the attempt to determine which slit the photon passes through with the observation of its position coordinate q. On the other hand the observation of the interference fringes corresponds to the observation of its momentum p.§ Since the reader will ask himself what happens in the case of a single slit, we consider this case in Example 1.2.

Example 1.2: The Single-Slit Experiment
Discuss the uncertainties of the canonical variables in relation to the diffraction fringes observed in a single-slit experiment.

Solution: Let light of wave-length λ fall vertically on a diaphragm S_1 with slit AB as shown schematicaly in Fig. 1.7.

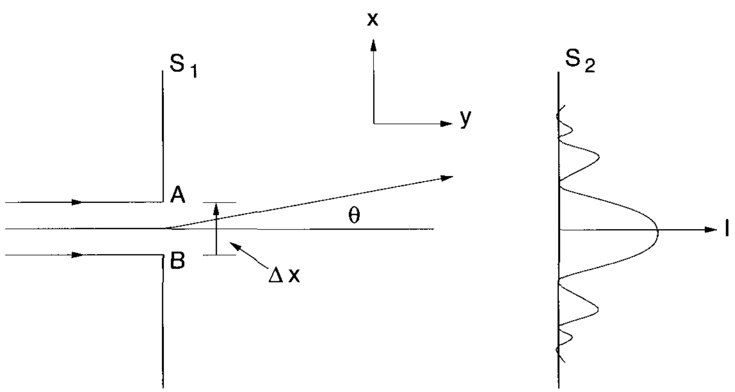

Fig. 1.7 Schematic arrangement of the single-slit experiment.

On the screen S_2 one then observes a diffraction pattern of alternately bright and dark fringes, in the

‡See, for instance, the discussion in A. Messiah [195], Vol. I, Sec. 4.4.4.

§Considerable discussion can be found in A. Rae [234].

figure indicated by maxima and minima of the light intensity I. As remarked earlier, the fringes are formed by interference of rays traversing different paths from the source to the observation screen. Before we enter into a discussion of uncertainties, we derive an expression for the intensity I. Since the derivation is not of primary interest here, we resort to a (still somewhat cunbersome) trick justification, which however can also be obtained in a rigorous way.¶ We subdivide the distance $AB = \triangle x$ into N equal pieces $AP_1, P_1P_2, \ldots$, as indicated in Fig. 1.8.

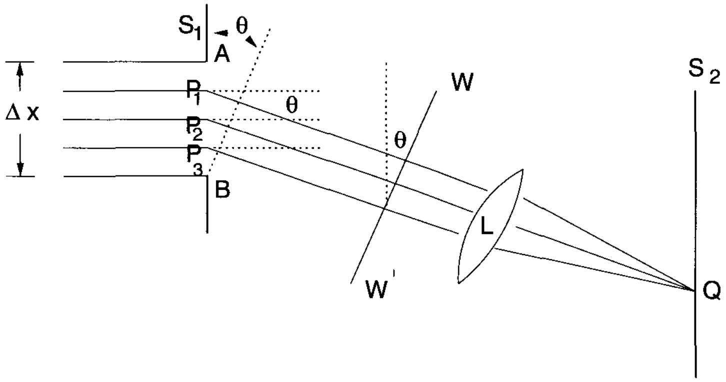

Fig. 1.8 The wave-front WW'.

We consider rays deflected by an angle θ with wave-front WW' and bundled by a lense L and focussed at a point Q on the screen S_2. Since WW' is a wave-front, all points on it have the same phase, so that light sent out from a source at Q reaches every point on WW' at the same time and across equal distances. Hence a phase difference at Q can be attributed to different path lengths from $P_1, P_2, \ldots$ to WW'. Considering two paths from neighbouring points P_i, P_j along AB, the difference in their lengths is $\triangle x \sin\theta/N$. In the case of a wave having the shape of the function

$$\sin kr = \sin \frac{2\pi}{\lambda} r,$$

this implies a phase difference given by

$$\delta_N = \frac{2\pi}{\lambda}\frac{\triangle x}{N}\sin\theta. \tag{1.20}$$

Just as we can represent an amplitude r having phase θ by a vector $\mathbf{r}$, i.e. $\mathbf{r} \rightarrow |\mathbf{r}|\exp(i\theta)$, we can similarly imagine the wave at Q, and this means its amplitude and phase, as represented by a vector, and similarly the wave of any component of the ray passing through $AP_1, P_1P_2, \ldots$. If we represent their effects at Q by vectors of equal moduli but different directions, their sum is the resultant OP_N as indicated in Fig. 1.9. In the limit $N \rightarrow \infty$ the N vectors produce the arc of a circle. The angle δ between the tangents at the two ends is the phase difference of the rays from the edges of the slit:

$$\delta = 2\alpha = \lim_{N\rightarrow\infty} N\delta_N = \frac{2\pi}{\lambda}\triangle x \sin\theta. \tag{1.21}$$

If all rays were in phase, the amplitude, given by the length of the arc OQ, would be given by the chord OQ. Hence we obtain for the amplitude A at Q if A_0 is the amplitude of the beam at the slit:

$$A = A_0 \frac{\text{length of chord } OQ}{\text{length of arc } OQ} = A_0 \frac{2a\sin\alpha}{a\,2\alpha} = A_0\frac{\sin\alpha}{\alpha}. \tag{1.22}$$

¶S. G. Starling and A. J. Woodall [260], p. 664. For other derivations see e.g. A. Brachner and R. Fichtner [32], p. 52.

The intensity at the point Q is therefore

$$I_\theta = I_0\left(\frac{\sin\alpha}{\alpha}\right)^2,$$

where from Eq. (1.21)

$$\alpha = \frac{\pi}{\lambda}\Delta x \sin\theta = \frac{k}{2}\Delta x \sin\theta.$$

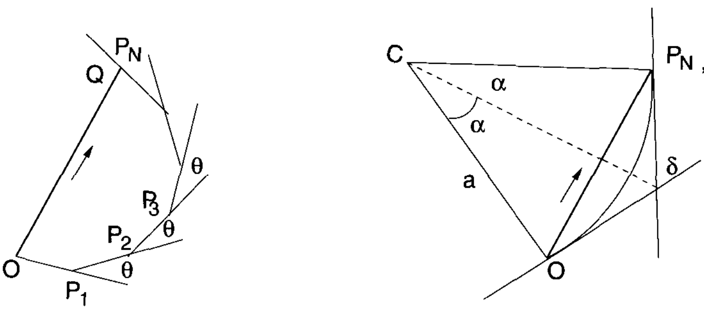

Fig. 1.9 The resultant OP_N of N equal vectors with varying inclination.

Thus the intensity at the point Q is

$$I_\theta = I_0\frac{\sin^2(k\Delta x\sin\theta/2)}{(k\Delta x\sin\theta/2)^2}. \tag{1.23}$$

The maxima of this distribution are obtained for

$$\frac{1}{2}k\Delta x\sin\theta = (2n+1)\frac{\pi}{2},\ \text{ i.e. for }\ \Delta x\ \sin\theta = (2n+1)\frac{\pi}{k} = (2n+1)\frac{\lambda}{2} \tag{1.24a}$$

and minima for

$$\frac{1}{2}k\Delta x\sin\theta = n\pi,\ \text{ i.e. for }\ \Delta x\ \sin\theta = n\lambda. \tag{1.24b}$$

The maxima are not exactly where only the numerator assumes extremal values, since the variable also occurs in the denominator, but nearby.

We return to the single-slit experiment. Let the light incident on the diaphragm S_1 have a sharp momentum $p = h/\lambda$. When the ray passes through the slit the position of the photon is fixed by the width of the slit Δx, and afterwards the photon's position is even less precisely known. We have a situation which — for the observation on the screen S_2 is a past (the uncertainty relation does not refer to this past with $p_x = 0$, rather to the position and momentum later; for the situation of the past $\Delta x\Delta p$ is less than h). The above formula (1.23) gives the probability that after passing through the slit the photon appears at some point on the screen S_2. This probability says, that the photon's momentum component p_x after passing through the slit is no longer zero, but indeterminate. It is not possible to predict at which point on S_2 the photon will appear (if we knew this, we could derive p_x from this). The momentum uncertainty in the direction x can be estimated from the geometry of Fig. 1.10, where θ is the angle in the direction to the first minimum:

$$\Delta p_x = 2p_x = 2p\sin\theta = \frac{2h}{\lambda}\sin\theta. \tag{1.25}$$

From Eq. (1.24b) we obtain for the angle θ in the direction of the first minimum

$$\Delta x\ \sin\theta = \lambda,$$

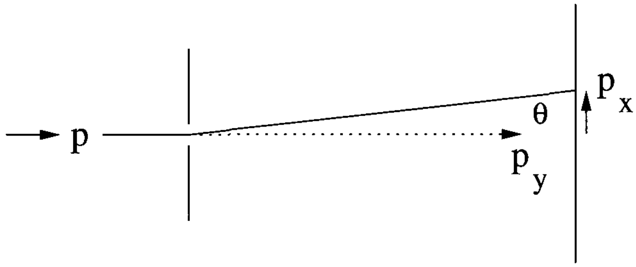

Fig. 1.10 The components of momentum p.

so that

$$\triangle x \, \triangle p_x = 2h.$$

If we take the higher order minima into account, we obtain $\triangle x \triangle p_x = 2nh$, or

$$\triangle x \, \triangle p_x \geq h.$$

We see that as a consequence of the indeterminacy of position and momentum, one has to introduce probability considerations. The limiting value of the uncertainty relation does not depend on how we try to measure position and momentum. It does also not depend on the type of particle (what applies to electromagnetic waves, applies also to particle waves).

1.4.1 Further thought experiments

Another experiment very similar to that described above is the attempt to localize a particle by means of an idealized microscope consisting of a single lense. This is depicted schematically in Fig. 1.11.

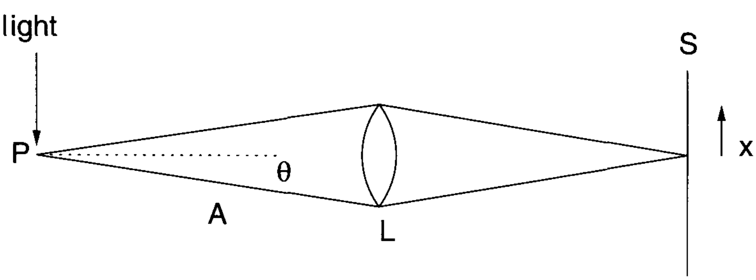

Fig. 1.11 Light incident as shown.

The resolving power of a lense L is determined by the separation $\triangle x$ of the first two neighbouring interference fringes, i.e. the position of a particle is at best determinable only up to an uncertainty $\triangle x$. Let θ be one half of the angle as shown in Fig. 1.11, where P is the particle. We allow light to fall in the direction of $-\mathbf{x}$ on the particle, from which it is scattered. We assume a quantum of light is scattered from P through the lense L to S where it is focussed and registered on a photographic plate. For the resolving power $\triangle x$ of the lense one can derive a formula like Eqs. (1.24a), (1.24b) . This is derived in books on optics, and hence will not be verified here, i.e.[||]

$$\triangle x \simeq \frac{\lambda}{2\sin\theta}. \tag{1.26a}$$

The precise direction in which the photon with momentum $p = h/\lambda$ is scattered is not known. However, after scattering of the photon, for instance along PA in Fig. 1.11, the uncertainty in its x-component is

$$\triangle p_x = 2p\sin\theta = \frac{2h}{\lambda}\sin\theta \tag{1.26b}$$

(prior to scattering the x-components of the momenta of the particle and the photon may be known precisely). From Eqs. (1.26a), (1.26b) we obtain again

$$\triangle x \, \triangle p_x \sim h.$$

The above considerations lead to the question of what kind of physical quantities obey an uncertainty relation. For instance, how about momentum and kinetic energy T? Apparently there are "*compatible*" and "*incompatible*" quantities, the latter being those subjected to an uncertainty relation. If the momentum p_x is "sharp", meaning $\triangle p_x = 0$, then also $T = {p_x}^2/2m$ is sharp, i.e. T and p_x are compatible. In the case of angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, we have

$$|\mathbf{L}| = |\mathbf{r}||\mathbf{p}'| = rp',$$

where $p' = p\sin\phi$. As one can see, r and p' are perpendicular to each other and thus can be sharp simultaneously. If p' lies in the direction of x, we have

$$\triangle x \, \triangle p' \geq h,$$

where now $\triangle x = r\triangle\varphi$, φ being the azimuthal angle, i.e.

$$r\triangle\varphi \, \triangle p' \geq h, \quad \text{i.e.} \quad \triangle L \, \triangle\varphi \geq h.$$

Thus the angular momentum $\mathbf{L}$ is not simultaneously exactly determinable with the angle φ. This means, when $\mathbf{L}$ is known exactly, the position of the object in the plane perpendicular to $\mathbf{L}$ is totally indeterminate.

Finally we mention an uncertainty relation which has a meaning different from that of the relations considered thus far. In the relation $\triangle x \, \triangle p_x \geq 0$ the

[||]See, for instance, N. F. Mott, [199], p. 111. In some books the factor of "2" is missing; see, for instance, S. Simons [251], p. 12.

quantities $\triangle x, \triangle p_x$ are uncertainties at one and the same instant of time, and x and p_x cannot assume simultaneously precisely determined values. If, however, we consider a *wave packet*, such as we consider later, which spreads over a distance $\triangle x$ and has *group velocity* $v_G = p/m$, the situation is different. The energy E of this wave packet (as also its momentum) has an uncertainty given by

$$\triangle E \approx \frac{\partial E}{\partial p}\triangle p = v_G \triangle p.$$

The instant of time t at which the wave packet passes a certain point x is not unique in view of the wave packet's spread $\triangle x$. Thus this time t is uncertain by an amount

$$\triangle t \approx \frac{\triangle x}{v_G}.$$

It follows that

$$\triangle t\,\triangle E \approx \triangle x\,\triangle p \geq h. \tag{1.27}$$

Thus if a particle does not remain in some state of a number of states for a period of time longer than $\triangle t$, the energy values in this state have an indeterminacy of $|\triangle E|$.

1.5 Bohr's Complementarity Principle

Vaguely expressed the complementarity principle says that two canonically conjugate variables like position coordinate x and the the associated canonical momentum p of a particle are related in such a way that the measurement of one (with uncertainty $\triangle x$) has consequences for the measurement of the other. But this is essentially what the uncertainty relation expresses. Bohr's complementarity principle goes further. Every measurement we are interested in is performed with a macroscopic apparatus at a microscopic object. In the course of the measurement the apparatus interferes with the state of the microscopic object. Thus really one has to consider the combined system of both, not a selected part alone. The uncertainty relation shows: If we try to determine the position coordinate with utmost precision all information about the object's momentum is lost — precisely as a consequence of the disturbance of the microscopic system by the measuring instrument. The so-called Kopenhagen view, i.e. that of Bohr, is expressed in the thesis that the microscopic object together with the apparatus determine the result of a measurement. This implies that if a beam of light or electrons is passed through a double-slit (this being the apparatus in this case) the photons or electrons behave like waves precisely because under these observation conditions they are waves, and that on the other hand, when observed in a counter, they behave like a stream of particles because under these conditions they are particles. In fact, without performance of some measurement (e.g. at some electron) we cannot say anything about the object's existence. The Kopenhagen view can also be expressed by saying that a quantity is real, i.e. physical, only when it is measured, or — put differently — the properties of a quantum system (e.g. whether wave-like or corpuscular) depend on the method of observation. This is the domain of conceptual difficulties which we do not enter into in more detail here.*

1.6 Further Examples

Example 1.3: The oscillator with variable frequency

Consider an harmonic oscillator (i.e. simple pendulum) with time-dependent frequency $\omega(t)$.
(a) Considering the case of a monotonically increasing frequency $\omega(t)$, i.e. $d\omega/dt > 0$, from ω_0 to ω', show that the energy E' satisfies the following inequality

$$E_0 \leq E' \leq \frac{\omega'^2}{\omega_0^2} E_0, \qquad (1.28)$$

where E_0 is its energy at deflection angle $\theta = \theta_0$. Compare the inequality with the quantum mechanical zero point energy of an oscillator.
(b) Considering the energy of the oscillator averaged over one period of oscillation (for slow, i.e. adiabatic, variation of the frequency) show that the energy becomes proportional to ω. What is the quantum mechanical interpretation of the result?

Solution: (a) The equation of motion of the oscillator of mass m and with variable frequency $\omega(t)$ is

$$m\ddot{x} + m\omega^2(t)x = 0,$$

where, according to the given conditions,

$$\frac{d\omega}{dt} \geq 0, \quad \omega = \omega_0 \text{ at } t = 0, \quad \omega = \omega' \text{ at } t = T,$$

i.e. $\omega(t)$ grows monotonically. Multiplying the equation of motion by $\dot{x}$ we can rewrite it as

$$\frac{d}{dt}\left[\frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2(t)x^2\right] - \frac{1}{2}mx^2\frac{d\omega^2}{dt} = 0.$$

The energy of the oscillator is

$$E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2(t)x^2, \quad \text{so that} \quad \frac{dE}{dt} = \frac{1}{2}mx^2\frac{d\omega^2}{dt} \geq 0, \qquad (1.29)$$

where we used the given conditions in the last step. On the other hand, dividing the equation of motion by ω^2 and proceeding as before, we obtain

$$\frac{\dot{x}}{\omega^2}[m\ddot{x} + m\omega^2(t)x] = 0, \quad \text{i.e.} \quad \frac{d}{dt}\left[\frac{1}{\omega^2}\frac{1}{2}m\dot{x}^2 + \frac{1}{2}mx^2\right] - \frac{1}{2}m\dot{x}^2\frac{d}{dt}\left(\frac{1}{\omega^2}\right) = 0,$$

*See e.g. A. Rae [234]; P. C. W. Davies and J. R. Brown [65].

or

$$\frac{d}{dt}\left(\frac{E}{\omega^2}\right) = \frac{1}{2}m\dot{x}^2\frac{d}{dt}\left(\frac{1}{\omega^2}\right) = -\frac{m\dot{x}^2}{\omega^3}\frac{d\omega}{dt} \leq 0, \tag{1.30}$$

where the inequality again follows as before. We deduce from the last relation that

$$\frac{1}{\omega^2}\frac{dE}{dt} - \frac{E}{\omega^4}\frac{d\omega^2}{dt} \leq 0, \quad \text{i.e.} \quad \frac{1}{E}\frac{dE}{dt} \leq \frac{1}{\omega^2}\frac{d\omega^2}{dt}. \tag{1.31}$$

Integrating we obtain

$$\int_{E_0}^{E'}\frac{dE}{E} \leq \int_{\omega_0^2}^{\omega'^2}\frac{d\omega^2}{\omega^2}, \quad \text{i.e.} \quad [\ln E]_{E_0}^{E'} \leq [\ln \omega^2]_{\omega_0^2}^{\omega'^2}, \quad \text{i.e.} \quad \frac{E'}{E_0} \leq \frac{\omega'^2}{\omega_0^2},$$

or

$$E' \leq \frac{\omega'^2}{\omega_0^2}E_0.$$

Next we consider the case of the harmonic oscillator as a simple pendulum in the gravitational field of the Earth with

$$\ddot{\theta} + \omega_0^2\theta \simeq 0, \quad \omega_0^2 = \frac{g}{l},$$

and we assume that — as explained in the foregoing — the length of the pendulum is reduced by one half so that

$$\omega'^2 = 2\frac{g}{l} = 2\omega_0^2.$$

Then the preceding inequality becomes

$$E' \leq 2E_0.$$

In shortening the length of the pendulum we apply energy (work against the tension in the string), maximally however E_0. Only in the case of the instantaneous reduction of the length at $\theta = 0$ (the pivot does not touch the string!) no energy is added, so that in this case $E' = E_0$, i.e.

$$E_0 \leq E' \leq 2E_0.$$

We can therefore rewrite the earlier inequality as

$$E_0 \leq E' \leq \frac{\omega'^2}{\omega_0^2}E_0.$$

Just as the equality on the left applies in the case of an instantaneous increase of the frequency (shortening of pendulum string), so the equality on the right applies to $\theta = \theta_{\text{max}}$. In *classical physics* we have

$$E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2x^2.$$

If no energy is added, but ω^2 is replaced by $2\omega^2$, then x changes, and also $\dot{x}$, i.e. x becomes shorter and $\dot{x}$ becomes faster. The quantum mechanical expression for the energy of the oscillator in its ground state is the zero point energy $E = \hbar\omega/2$. Here in *quantum physics* we cannot change ω without changing E. This means if we double ω instantaneously (i.e. in a time interval $\Delta t \to 0$) without addition of energy (to $\hbar\omega/2$), then the result $E' = \hbar\omega$ is incorrect by $\Delta E = \hbar\omega/2$. We cannot have simultaneously $\Delta t \to 0$ and error $\Delta E = 0$.

(b) The classical expression for E contains ω quadratically, the quantum mechanical expression is linear in ω. We argue now that we can obtain an expression for $E_{\text{classical}}$ by assuming that $\omega(t)$ varies very little (i.e. "adiabatically") within a period of oscillation of the oscillator, T. Classical mechanics is deterministic (i.e. the behaviour at time t follows from the equation of motion and the initial conditions); hence for the consideration of a single mass point there is no reason for an averaging over a period, unless we are not interested in an exact value but, e.g. in the average

$$\left\langle \frac{1}{2}mx^2 \right\rangle = \frac{1}{T}\int_0^T \frac{1}{2}mx^2(t)dt. \tag{1.32}$$

If ω is the frequency of $x(t)$, i.e. $x(t) \propto \cos\omega t$ or $\sin\omega t$ depending on the initial condition, then $\dot{x}^2(t) = \omega^2 x^2$ and hence

$$\left\langle \frac{1}{2}m\omega^2 x^2 \right\rangle = \left\langle \frac{1}{2}m\dot{x}^2 \right\rangle = \frac{1}{2}E$$

(as follows also from the virial theorem). If we now insert in the equation for dE/dt, i.e. in Eq. (1.29), for $mx^2/2$ the mean value

$$\left\langle \frac{1}{2}mx^2 \right\rangle = \frac{1}{2}\frac{E}{\omega^2},$$

we obtain

$$\frac{dE}{dt} = \left\langle \frac{1}{2}mx^2 \right\rangle \frac{d\omega^2}{dt} = \frac{E}{2\omega^2}\frac{d\omega^2}{dt}, \quad \text{or} \quad \frac{dE}{E} = \frac{1}{2}\frac{d\omega^2}{\omega^2} = \frac{d\omega}{\omega},$$

and hence

$$\frac{E}{\omega} = \text{const.}$$

In quantum mechanics with $E = \hbar\omega(n+1/2)$ this implies $\hbar(n+1/2) = \text{const.}$, i.e. $n = \text{const.}$ This means, with slow variation of the frequency the system remains in state n. This is an example of the so-called *adiabatic theorem of Ehrenfest*, which formulates this in a general form.[†]

Example 1.4: Angular spread of a beam

A dish-like aerial of radius R is to be designed which can send a microwave beam of wave-length $\lambda = 2\pi\hbar/p$ from the Earth to a satellite. Estimate the angular spread θ of the beam.

Solution: Initially the photons are restricted to a transverse spread of length $\triangle x = 2R$. From the uncertainty relation we obtain the uncertainty $\triangle p_x$ of the transverse momentum p_x as $\triangle p_x \simeq \hbar/2R$. Hence the angle θ is given by

$$\theta \simeq \frac{\triangle p_x}{p} = \frac{\hbar}{2R}\left(\frac{\lambda}{2\pi\hbar}\right) = \frac{\lambda}{4\pi R}.$$

[†]See e.g. L. Schiff [243], pp. 25 - 27.