Chapter 1
Theoretical Background of Quantum Metrology

Abstract This chapter outlines the history of quantum mechanics and presents its fundamental formulas: the Schrödinger equation with the interpretation of the wave function, the Pauli exclusion principle, and the Heisenberg uncertainty principle. The latter is illustrated with sample numerical calculations. We briefly discuss the application of quantum effects in metrology, and present and compare the limits of accuracy and resolution of classical and quantum standards. Prospects for a new system of units are discussed as well.

1.1 Introduction

Measurement consists in comparing the measured state A_x of a quantity to its state A_{ref} considered a reference state, as shown schematically in Fig. 1.1. Thus, the accuracy of the measurement cannot be better than the accuracy of the standard.

For many years metrologists have been working on the development of standards that would only depend on fundamental physical constants and atomic constants. With such standards units of measurement can be realized on the basis of quantum phenomena. One of the directions of research in metrology is the creation of a new system of measurement, based on a set of quantum and atomic standards, that would replace the classical SI system.

In the present chapter we shall focus on measures and the development of the system of units of measurement. We shall discuss the history of measurement standards and present in detail the currently used International System of Units (SI). The set of the base units of the SI system of measurement will be discussed as well. The following chapters present the quantum phenomena that are the most commonly used in metrology: the Josephson effect is discussed in Chap. 4, the quantum Hall effect in Chap. 6, and the tunneling of single electrons in Chap. 8. These three phenomena are considered of particular importance not only for electrical metrology,

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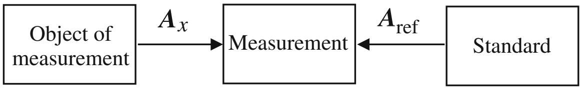

Fig. 1.1 Measurement: a comparison between the object and standard

but also for science as a whole. For his theoretical studies predicting the effect of voltage quantization Brian David Josephson was awarded the Nobel Prize in 1973, and Klaus von Klizing received the Nobel Prize in 1985 for his discovery of the quantum Hall effect.

Standards for a quantum system of measurements based on quantum mechanical phenomena have been implemented in the past 25 years. Quantum phenomena are described in terms of concepts of quantum mechanics. The beginning of quantum mechanics is conventionally set at 1900, when Max Planck proposed a new formula for the intensity of emission of electromagnetic radiation in the thermal and visible wavelength ranges of the spectrum. In his analysis Planck assumed that the energy changed by quanta proportional to a constant denoted as h, which was later named the Planck constant. The dependence proposed by Planck described the measured emission of electromagnetic radiation much better than the models in use at that time, based on the rules of classical physics. As a set of rules and formulas quantum mechanics was developed in the 1920s by Erwin Schrödinger, who formulated the Schrödinger equation, and Werner Heisenberg, the author of the uncertainty principle, with major contributions by Louis de Broglie, Max Born, Niels Bohr, Paul Dirac, and Wolfgang Pauli. Unlike classical physics, quantum mechanics often leads to renounce the common-sense comprehension of physical phenomena and utterly astounds the researcher or reader. One of its latest surprises is the observation of electric current flowing simultaneously (!) in both directions on the same way in the circuit [4]. As Niels Bohr, the author of the model of the hydrogen atom, said: *Anyone who is not shocked by quantum theory probably has not understood it.*

Quantum mechanical phenomena are employed in at least three fields of metrology:

- The construction of quantum standards of units of physical quantities: standards for electrical quantities such as voltage, electrical resistance or electrical current, and non-electrical standards, including the atomic clock and the laser standard for length;
- The determination of the physical limits of measurement precision by the Heisenberg uncertainty principle;
- The construction of extremely sensitive electronic components: the magnetic flux sensor referred to as SQUID (Superconducting Quantum Interference Device) and the SET transistor based on single electron tunneling.

1.2 Schrödinger Equation and Pauli Exclusion Principle

The development of quantum mechanics was preceded by a discovery by *Max Planck* in 1900. On the basis of measurements of the intensity of black-body radiation Planck derived a formula based on the assumption that the energy was exchanged in a noncontinuous manner between particles and radiation, and emitted in quanta proportional to a constant, which is now known as the Planck constant h ($h = 6.626 \times 10^{-34}$ J s), and the radiation frequency f:

$$E = h \times f. \tag{1.1}$$

The results of measurements of the energy density of the radiation as a function of the temperature and frequency in the thermal, visible and ultraviolet ranges of the spectrum (spanning the wavelengths from 200 nm to 10 μm) could not be explained by the rules of classical physics. Established on the basis of classical physics, the Rayleigh-Jeans formula for the energy density, although formally correct, only described accurately the studied phenomenon in the far infrared spectral range, i.e., for wavelengths above 5 μm. For shorter wavelengths the results obtained from the Rayleigh-Jeans formula diverged so much from the measurement data that the theoretical dependence in this range, predicting infinite energy density, was named the ultraviolet catastrophe. Only the formula derived by Planck on the assumption that energy was quantized corresponded well to the measurement data in the whole wavelength range [7], as indicated by the plot in Fig. 1.2.

The Planck law is expressed as a dependence $u(f, T)$ of the spectral radiant emission on the frequency f and temperature T (1.2), or a dependence $u(\lambda, T)$ of the spectral radiant emission on the wavelength λ and temperature T:

$$u(f, T) = \frac{4hf^3}{c^3} \frac{1}{\exp\left(\frac{hf}{k_B T}\right) - 1}, \tag{1.2}$$

where $u(f, T)$ is the spectral radiant emission of a perfect black body, f is the radiation frequency, T—the absolute temperature of the black body, h—the Planck constant, k_B—the Boltzmann constant, and c—the speed of light in vacuum.

The Planck lecture on the subject, presented at a meeting of the Berliner Physikalische Gesellschaft on December 14, 1900, is considered the beginning of quantum mechanics. Five years later, in 1905, *Albert Einstein*, analyzing the photoelectric effect, came to the conclusion that not only the emitted energy, but also the energy E of absorbed light was quantized. Einstein was the first to affirm that the energy of light was carried in portions hf proportional to the frequency f and to the Planck constant [2]. Contrary to the common opinion at that time, Einstein presented light as discrete. This result of theoretical considerations was received with general disbelief. When the quantum nature of the energy of light was confirmed experimentally by the American physicist Robert A. Millikan in 1915, he himself was very surprised at that result. Moreover, to light quanta, later named

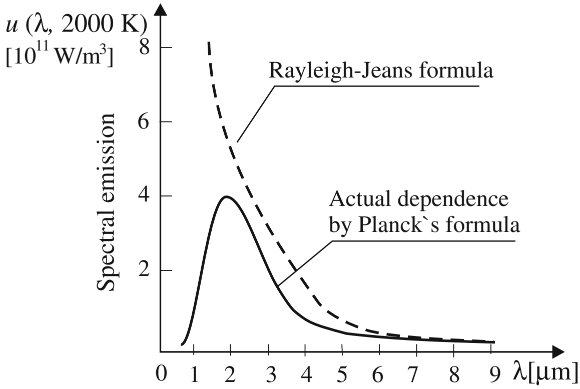

Fig. 1.2 Spectral radiant emission of a black body in the thermal and visible spectral ranges at the temperature of 2,000 K according to the Rayleigh-Jeans formula (*dashed line*) and by the Planck formula (*solid line)* [6]

photons, Einstein attributed properties of material particles with zero rest mass. Evidence for the quantum character of light was provided, among others, by the experiments by Walther Bothe and Arthur H. Compton.

Einstein's studies on the photoelectric effect were so momentous for theoretical physics that they brought him the Nobel Prize in 1921. Albert Einstein is often portrayed as a skeptic of quantum mechanics, in particular its probabilistic description of phenomena. However, by his studies on the photoelectric effect (1905) and the specific heat of solids (1907) he unquestionably contributed to the development of quantum mechanics. In his publication on specific heat Einstein introduced elements of the quantum theory to the classical theory of electrical and thermal conduction in metals, which was proposed by Paul Drude in 1900.

A hypothesis that the whole matter had a particle-wave nature was put forward by *Louis de Broglie* in 1924 in his PhD Thesis, in which he considered the nature of light [5, 8]. At that time it was already known that light exhibited the properties of both particles and waves. The evidence provided by experiments included the observation of the bending of light rays in the gravitational field of stars, an effect predicted by Einstein. De Broglie's hypothesis proposed that, if light had the properties of particles, besides those of waves, it might be that also the elementary particles that constituted matter had characteristics of both particles and waves. According to de Broglie, the movement of a material particle is associated with a wave of length λ and frequency f:

$$\lambda = \frac{h}{p} = \frac{h}{mv}, \quad f = \frac{E}{h}, \tag{1.3}$$

where λ is the wavelength corresponding to the position of the particle, p the momentum of the particle, m its mass, E its energy, and h the Planck constant.

The movement of an electron at a speed of 10^3 m/s is associated with a wave of wavelength $\lambda \approx 7 \times 10^{-7}$ m (ultraviolet radiation), as calculated from (1.3). The movement of a neutron with the same speed (10^3 m/s) is associated with a wave of wavelength $\lambda \approx 4 \times 10^{-13}$ m. In other words, a neutron moving with that speed can be considered a *de Broglie wave* with a wavelength of 4×10^{-13} m. Similar wavelengths are characteristic of cosmic rays. Particles with a mass much larger than that of the neutron, even when moving at a much lower speed (1 m/s), would be associated with waves so short that their measurement would be impossible. Thus, the wave properties of such particles cannot be confirmed. For example, a particle with a hypothetic mass of 10^{-3} g and a velocity of 1 m/s would correspond to a de Broglie wave of wavelength $\lambda \approx 7 \times 10^{-28}$ m. Since neither waves with such a wavelength, nor elementary particles with a mass of the order of 1 mg have ever been observed, we do not know if they exist.

A good example of the particle-wave duality of matter is the electron, discovered by *John J. Thomson* in 1896 as a particle with an electric charge that was later established to be $e = 1.602 \times 10^{-19}$ C, and a mass $m = 9.11 \times 10^{-31}$ kg. The wave properties of the electron were demonstrated experimentally by the diffraction of an electron beam passing through a metal foil, observed independently by George P. Thomson (son of J.J. Thomson, the discoverer of the electron), P.S. Tartakovsky [8] and the Polish physicist Szczepan Szczeniowski.

One of the milestones in the history of physics, the Schrödinger equation was formulated (not derived) by the Austrian physicist *Erwin Schrödinger* in 1926 on the speculative basis by analogy with the then known descriptions of waves and particles. Since the validity of the formula has not been challenged by any experiment so far, it is assumed that the Schrödinger equation is true. If the Heisenberg uncertainty principle sets the limits to the accuracy with which parameters of a particle can be determined, the Schrödinger equation describes the state of an elementary particle. The *Schrödinger equation* features a function referred to as the wave function or state function and denoted as Ψ (*psi*), and expresses its complex dependence on time and the position coordinates of the particle:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + A\Psi = j\hbar\frac{\partial\Psi}{\partial t}, \tag{1.4}$$

where Ψ is the wave function, A a function of time and the coordinates of the particle, m the mass of the particle, t denotes time, ∇ the Laplace operator, $\hbar = h/2\pi$ is reduced the Planck constant, i.e. the Planck constant divided by 2π, and j is the imaginary unit.

When the function A is independent of time, it expresses the potential energy of the particle. In such cases the Schrödinger equation takes the form:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + A\Psi = E\Psi, \tag{1.5}$$

where A is the potential energy of the particle, and E denotes its total energy.

A physical interpretation of the wave function was first provided in 1926 by *Max Born* (born in Wroclaw, then Breslau, in 1882). The wave function describes the probability that the particle is present within a certain region, specifically in a volume dV. The probability is proportional to the square of the module of the wave function:

$$p = k|\Psi|^2 \mathrm{d}V, \tag{1.6}$$

where p denotes the probability, k is the proportionality coefficient, and V the volume of space available to the particle.

Pauli's exclusion principle says that in an atom no two electrons can have the same quantum state i.e. no two electrons can have the same set of four quantum numbers. The Pauli exclusion principle must be taken into account when separate atoms or nanostructures are analyzed (2-dimensional electron gas—see Chap. 6, nanostructures—see Chap. 7 and single electron tunneling—see Chap. 8).

1.3 Heisenberg Uncertainty Principle

A description of elementary particles which was equivalent to the Schrödinger equation had been proposed before, in 1925, by the German physicist *Werner Heisenberg* (who was 24 years old at that time!). Two years later Heisenberg formulated the uncertainty principle [3, 8], which is one of the foundations of quantum mechanics. The now famous relations expressing the uncertainty principle were proposed by Heisenberg in 1927 in an article *Über den Inhalt der anschaulichen quantentheoretischen Kinematik und Mechanik*. The uncertainty principle is closely related to the particle-wave duality of matter. It defines the limits of accuracy with which the state of a particle can be determined. The uncertainty principle has nothing to do with the accuracy of the instruments used for the measurement. When the position x of an electron, regarded as a particle, is established with an uncertainty (or margin of error, in the language of metrology) Δx, the state of this electron can also be represented in the wave image as a wave beam consisting of waves with different wavelengths. The electron is assigned a wavelength λ, the value of which is related to the momentum of the electron. According to the de Broglie formula:

$$\begin{gathered} \lambda = \frac{h}{p} \\ p = mv, \end{gathered} \tag{1.7}$$

where m is the mass of the electron, and v its speed.

Along the segment Δx corresponding to the uncertainty in the position of the particle a wave has n maximums and the same number of minimums:

$$\frac{\Delta x}{\lambda} = n. \tag{1.8}$$

A wave beam with zero amplitude beyond the segment Δx must include waves that have at least (n + 1) minimums and maximums along this segment:

$$\frac{\Delta x}{\lambda - \Delta\lambda} \geq n + 1. \tag{1.9}$$

From (1.8) and (1.9) it follows that:

$$\frac{\Delta x \times \Delta\lambda}{\lambda^2} \geq 1.$$

From the de Broglie formula we get:

$$\frac{\Delta\lambda}{\lambda^2} = \frac{\Delta p}{h}.$$

Finally, we obtain the formula for the *uncertainty principle*:

$$\Delta x \times \Delta p \geq \hbar/2, \tag{1.10}$$

where, $\hbar = h/2\pi$—reduced the Planck constant.

According to the (1.10), the product $\Delta x \times \Delta p$ of the uncertainty Δx in the position of the particle (e.g. electron) in one dimension and the uncertainty Δp in its momentum p in simultaneous determination of x and p (which is very important to note) is not less than the reduced Planck constant divided by 2. This means that even in the most accurate measurements or calculations for simultaneous determination of the position x of the particle and its momentum p, if the uncertainty Δx in the position is reduced, the uncertainty Δp in the momentum must increase, and vice versa. When the position of the particle is defined in three dimensions by coordinates x, y, z, a set of three inequalities applies in place of the single inequality (1.10):

$$\begin{aligned} \Delta x \times \Delta p_x &\geq \hbar/2 \\ \Delta y \times \Delta p_y &\geq \hbar/2 \\ \Delta z \times \Delta p_z &\geq \hbar/2. \end{aligned} \tag{1.11}$$

The uncertainty principle is of much practical importance in nanometer-sized structures. For example, if the uncertainty in the determination of the position of the electron is 2×10^{-10} m (the order of magnitude corresponding to the dimensions of an atom), according to the formula (1.10) the velocity of the electron can be determined with an uncertainty Δv:

$$\Delta x\,(m \times \Delta v) \geq \hbar/2$$

$$\Delta v \geq \frac{h}{4\pi\, m\, \Delta x} = \frac{6.626 \times 10^{-34}\,\text{Js}}{4\pi \times 9.1 \times 10^{-31}\,\text{kg} \times 2 \times 10^{-10}\,\text{m}} = 2.9 \times 10^{5}\,\text{m/s}.$$

This is a wide range, about three times wider than the velocity of the electron, v_{th}, related to the thermal energy k_BT at room temperature ($v_{\text{th}} \approx 10^5$ m/s).

If we give up the simultaneous determination of the parameters of the motion of the particle and assume that its position is fixed, the formula (1.12) below will provide the limits to the uncertainty ΔE in the energy of the particle and the uncertainty Δt in its lifetime or the observation time:

$$\Delta E \times \Delta t \geq \hbar/2. \tag{1.12}$$

For instance, let us calculate the time Δt necessary for a measurement of energy with the uncertainty $\Delta E = 10^{-3}$ eV = 1.6×10^{-22} J:

$$\Delta t \geq \frac{\hbar}{2\,\Delta E} = \frac{6.63 \times 10^{-34}}{4\pi \times 1.6 \times 10^{-22}} \approx 3.3 \times 10^{-13}\,\text{s} = 0.33\,\text{ps}.$$

1.4 Limits of Measurement Resolution

A question worth considering in measurements of low electrical signals by means of quantum devices is the existence of limits to the energy resolution of the measurement. Can signals be measured in arbitrarily small ranges? By the energy resolution we understand here the amount of energy or the change in energy that is possible to measure with a measuring instrument. Well, the limits of measurement resolution are not specified. Its physical limitations result from:

- The Heisenberg uncertainty principle in the determination of parameters of elementary particles;
- The quantum noise of the measured object, which emits and/or absorbs electromagnetic radiation;
- The thermal noise of the measured object.

The thermal noise power spectral density in an object at an absolute temperature T is described by the Planck equation:

$$\frac{P(T,f)}{\Delta f} = hf + \frac{hf}{\exp(\frac{hf}{k_BT}) - 1}, \tag{1.13}$$

where k_B is the Boltzmann constant.

The Planck equation (1.13) takes two extreme forms depending on the relationship between the thermal noise energy k_BT and the quantum hf of energy of electromagnetic radiation. For $k_B T \gg hf$ the Planck equation only includes the thermal noise component and takes the form of the Nyquist formula:

$$E(T) = \frac{P(T)}{\Delta f} \cong k_B T. \tag{1.14}$$

For $k_B T \ll hf$ the Planck equation only includes the quantum noise:

$$E(f) = \frac{P(f)}{\Delta f} \cong hf. \tag{1.15}$$

It can be noticed that thermal noise plays a dominant role in the description of the spectral power at low frequencies, whereas quantum noise predominates at high frequencies. The frequency f for which both components of the spectral noise power are equal, $k_B T = hf$, depends on the temperature; for example, $f = 6.2 \times 10^{12}$ Hz at the temperature of 300 K, and $f = 56$ GHz at 2.7 K, which is the temperature of space [3].

The (1.15) also describes energy as a physical quantity quantized with an uncertainty conditioned by the uncertainty in the measured frequency (currently of the order of 10^{-16}), and the accuracy with which the Planck constant is determined (presently of the order of 10^{-9}).

Below we present an attempt to estimate the lower bound of the measurement range in the measurement of electric current. Electric current is a flow of electrons, and its intensity in the conductor is defined as the derivative of the flowing electric charge $Q(t)$ with respect to time t, or as the ratio of the time-constant electric charge Q to the time t over which the charge is transferred:

$$I = \frac{\mathrm{d}Q(t)}{\mathrm{d}t}. \tag{1.16}$$

On the microscopic scale we can consider, and, what is more important, record, the flow of single electrons and calculate the intensity of the related electric current. Thus, for example, the flow of one billion (10^9) of electrons over 1 s is a current of 1.6×10^{-10} A, or 160 pA. It is now possible to measure electric current of such intensity with present-day ammeters, and sometimes even with multimeters, which combine a number of measurement functions for different physical quantities. A flow of electric charge at a much lower rate, such as one electron per second or one electron per hour, will no longer be regarded as electric current. In this case it is preferable to consider the motion of individual electrons and count the flowing charges, since the averaging of individual electrons over time tends to be useless.

Sensors measuring physical quantities respond to the energy or change in energy of the signal. Thus, the sensitivity of the measurement is limited by the Heisenberg uncertainty principle. The best energy resolution to date has been achieved by SQUID sensors; its value, equal to $0.5h$, reaches the physical limit (see Chap. 5). In measurements of linear displacement the best linear resolution, of 10^{-6} Å $= 10^{-16}$ m, has been obtained with the X-ray interferometer [1]. This wonderful achievement in metrology is worth comparing with atomic dimensions: for example, the diameter of the copper atom is 3.61 Å, and that of the gold atom is 4.08 Å. In measurements of displacement and geometrical dimensions the best linear resolution, $\Delta a = 0.01$ Å = 10^{-12} m and $\Delta b = 0.1$ Å in vertical and horizontal measurements, respectively, has been obtained with the scanning tunneling microscope (STM) in the study of the atom arrangement on the surface of a solid (see Chap. 11). The operation of the STM is based on the quantum effect of electron tunneling through a potential barrier.

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