1.1 Quantization of Energy

The foundation of quantum mechanics was laid in 1900 with Max Planck's discovery of the quantized nature of energy. When Planck developed his formula for black body radiation he was forced to assume that the energy exchanged between a black body and its thermal (electromagnetic) radiation is not a continuous quantity but needs to be restricted to discrete values depending on the (angular-) frequency of the radiation. Planck's formula can explain – as we shall see – all features of the black body radiation and his finding is phrased in the following way:

Proposition 1.1 *Energy is quantized and given in units of* $E = \hbar\omega$

Here ω denotes the angular frequency $\omega = 2\pi\nu$. We will drop the prefix "angular" in the following and only refer to it as the frequency. We will also bear in mind the connection to the wavelength λ given by $c = \lambda\nu$, where c is the speed of light, and to the period T given by $\nu = \frac{1}{T}$.

If we compare the energy of the photon as given by special relativity $E = pc$ and quantum mechanics $E = \hbar\omega$ we get the momentum of the photon:

$$k = \frac{\omega}{c} \quad \Rightarrow \quad E = \hbar kc \quad \Rightarrow \quad p = \hbar k .$$

Momentum of the photon $\vec{p}_{\text{photon}} = \hbar\vec{k}$

Proposition (Bohr's complementarity principle)

Wave and particle are two aspects of describing physical phenomena, which are complementary to each other.

Depending on the measuring instrument used, either waves or particles are observed, but never both at the same time, i.e. wave- and particle-nature are not simultaneously observable.

1.2 Wave Properties of Matter

As we will see in this section, not only radiation, but also massive particles are in need of a more sophisticated description than given by classical mechanics. To associate microscopical (quantum) objects, as for example electrons, with idealized (especially localized) point-particles, carrying sharp momenta, is not only misleading, but simply wrong and can not account for all observed phenomena. A very important step towards a more complete description was Louis de Broglie's proposal of wavelike behaviour of matter in 1923, which he received the Nobel prize for in 1929.

1.2.1 Louis de Broglie's Hypothesis

In view of particle properties for light waves – photons – Louis de Broglie ventured to consider the reverse phenomenon, he proposed to assign wave properties to matter, which we will formulate here in the following way:

Proposition (Louis de Broglie's hypothesis)
To every particle with mass m, momentum $\vec{p}$ and energy E a wavelength of $\lambda_{\text{deBroglie}} = \frac{h}{|\vec{p}|} = \frac{h}{\sqrt{2mE}}$ is associated, where $E = E_{\text{kin}} = \frac{\vec{p}^2}{2m}$.

The above statement can be easily understood when assigning energy and momentum

$$E = \hbar\omega \quad \text{and} \quad p = \hbar k = \frac{h}{\lambda}$$

to matter in (reversed) analogy to photons. If we then express the wavelength λ through the momentum p and use the form of the kinetic energy $E = p^2/2m$ to write $p = \sqrt{2mE}$ we directly get the *de Broglie wavelength* $\lambda_{\text{deBroglie}}$ of massive particles.

In this connection the notion of *matter waves* was introduced. De Broglie's view was that there exists a *pilot wave* which leads the particle on definite trajectories. This point of view – wave *and* particle – being in contrast to Bohr's view leads, however, into serious difficulties as we shall see.

Note that above wave assignment was made for free particles, i.e. particles that are not subjected to any outer potential. The question whether the potential energy would influence his hypothesis was also raised by de Broglie and will be tangible when we con- sider Schrödinger's theory where also the nature of the waves becomes more evident in terms of Max Born's probability interpretation.

2. Electron Diffraction from a Crystal

To test his hypothesis de Broglie proposed an experiment with electrons. He observed that, electrons with a kinetic energy of several eV and mass $m_e = 0,5$ MeV would have a de Broglie wavelength of a few Å. For example, for an energy of 10 eV we obtain $\lambda_{\text{deBroglie}} = 3,9$ Å, which is the same order of magnitude as the lattice spacing of atoms in crystals, thus making it possible to diffract electrons from the lattice analogously to the diffraction of light from a grating.

The corresponding experiment has been performed by C.Davisson and L.Germer in 1927 and independently by G.P. Thomson. It involved electrons which were sent with appropriate velocity onto a nickel crystal with lattice spacing $d \cong 0,92$ Å, see Fig. 1.

The intensity of the outgoing electron beam was then measured for different angles, reproducing the diffraction pattern postulated by W.H.Bragg and (his son) W.L.Bragg for X-rays. The similarity of X-ray- and electron-diffraction can be seen in Fig. 2.

The Bragg condition for constructive interference is $\boxed{\sin\vartheta = \frac{n\lambda}{2d}}$, $n \in N$.

The observation of an intensity maximum of the diffraction (Bragg peak) for a scattering angle $\phi = 50^\circ$, which translates to the angle in the Bragg condition of $\Theta = 65^\circ$, gives us

$$\Rightarrow \quad \lambda = 2 \times 0,92\,\mathring{A} \times \sin 65^\circ = 1,67\,\mathring{A} \,,$$

which is in perfect accordance with the de Broglie wavelength for an acceleration voltage of $U = 54$ V used in this experiment.

The Davisson-Germer experiment thus helped to confirm the wavelike nature of matter

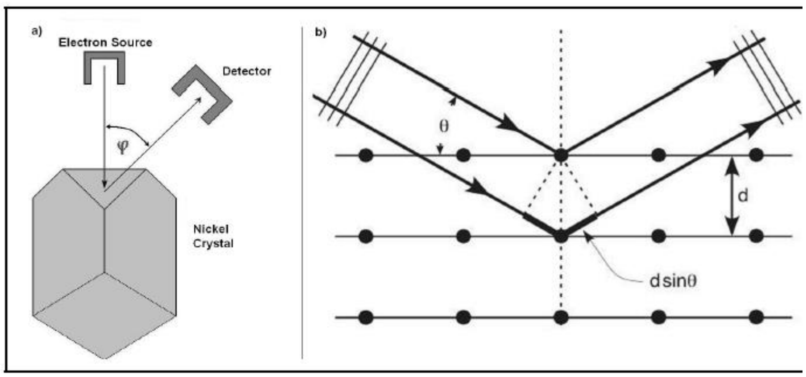

Figure 1.: Davisson-Germer Experiment: a) An electron beam is diffracted from a nickel crystal and the intensity of the outgoing beam is measured. b) Scheme of the Bragg diffraction from a crystal with lattice spacing *d*,

and to validate the claims of early quantum mechanics. Davisson and Thomson[6] were awarded the Nobel prize in 1937.

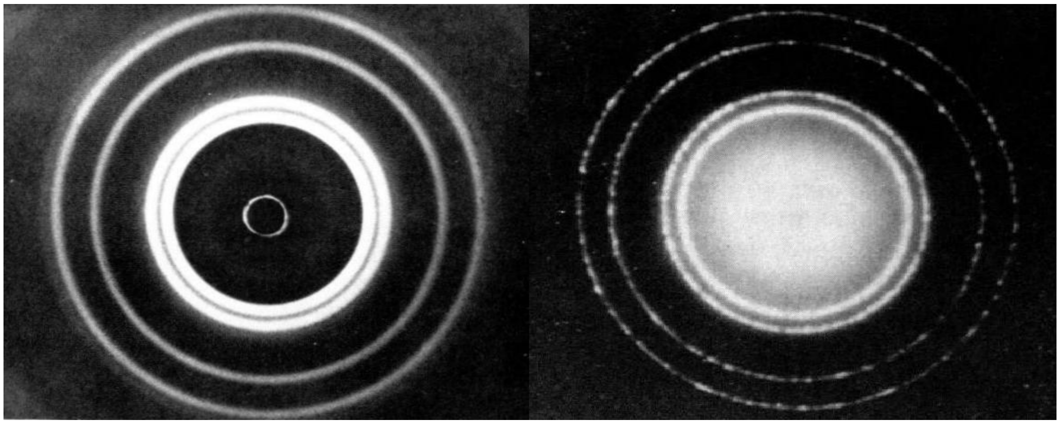

Figure 1.12: Comparison of X-ray- (left) and electron- (right) diffraction patterns caused by the same aperture, namely a small hole in an aluminium foil; pictures from Ref. [2]

3. Heisenberg's Uncertainty Principle

We now want to introduce a quantum mechanical principle, *Heisenberg's uncertainty principle* that is somehow difficult to grasp conceptually even though the mathematics behind is straightforward. Before we will derive it formally, which we will do in Sect. 2.6, we try to make it plausible by more heuristic means, namely by the *Heisenberg microscope*. The Gedankenexperiment of the Heisenberg microscope needs to be seen more as an example for the application of the uncertainty principle, than a justification of the principle itself.

3.1 Heisenberg's Microscope

Let's start by detecting the position of an electron by scattering of light and picturing it on a screen. The electron will then appear as the central dot (intensity maximum) on the screen, surrounded by bright and dark concentric rings (higher order intensity maxima/minima). Since the electron acts as a light source we have to consider it as an aperture with width d where we know that the condition for destructive interference is

$$\sin \varphi = \frac{n\lambda}{d} \, , \; n \in \mathrm{N} .$$

So following Eq. (1.23) the smallest length resolvable by a microscope is given by $d = \lambda / \sin \varphi$ and thus the *uncertainty of localization* of an electron can be written as

$$\Delta x = d = \frac{\lambda}{\sin \varphi} .$$

It seems as if we chose the wavelength λ to be small enough and $\sin \varphi$ to be big, then Δx could become arbitrarily small. But, as we shall see, the accuracy increases at the expense of the momentum accuracy. Why is that? The photons are detected on the screen but their direction is unknown within an angle φ resulting in an uncertainty of the electron's recoil within an interval Δ. So we can identify the momentum uncertainty (in the direction of the screen) of the photon with that of the electron

$$\Delta p_x^e = \Delta p_x^{\text{Photon}} = p^{\text{Photon}} \sin\phi = \frac{h}{\lambda} \sin\phi \,,$$

where we inserted the momentum of the photon $p^{\text{Photon}} = hk = h/\lambda$ in the last step.

Heisenberg's Uncertainty relation: $\Delta x \, \Delta p_x = h$

which he received the Nobel prize for in 1932. We will further see that the accuracy can be increased by a factor 4π and that the above relation can be generalized to the statement

$$\Delta x \, \Delta p_x \geq \frac{\hbar}{2}$$

This is a fundamental principle that has nothing to do with technical imperfections of the measurement apparatus. We can phrase the uncertainty principle in the following way:

Proposition

Whenever a position measurement is accurate (i.e. precise information about the current position of a particle), the information about the momentum is inaccurate – uncertain – and vice versa.

4. Energy–Time Uncertainty Principle

We now want to construct another uncertainty relation, the energy–time uncertainty, which describes the relation between the uncertainties Δt for the time a physical process lasts and ΔE for the respective energy. Consider for example a wave packet traveling along the x-axis with velocity v. It takes the time Δt to cover the distance Δx. We can thus write

energy: $E = \frac{p^2}{2m}$ velocity $v = \frac{\Delta x}{\Delta t}$

Calculating the variation ΔE of the energy E and expressing Δt from the right hand side of Eq. (1.26) by the velocity v and substituting $v = p/m$ we get

variation: $\Delta E = \frac{p}{m} \Delta p$ time period: $\Delta t = \frac{\Delta x}{v} = \frac{m}{p} \Delta x.$

The right hand side represents the period of time where the wave is localizable. When we now multiply Δt with ΔE we arrive at:

$$\Delta t \, \Delta E = \frac{m}{p} \Delta x \frac{p}{m} \Delta p = \Delta x \, \Delta p \geq \frac{\hbar}{2},$$

$$\Delta E \, \Delta t \geq \frac{\hbar}{2}$$

We can conclude that there is a fundamental complementarity between energy and time. An important consequence of the energy–time uncertainty is the finite "natural" width of the spectral line