Werner Heisenberg (1901–1976)
Established uncertainty principle

5

The Heisenberg uncertainty principle

5.1 Definition of uncertainty

Quantum mechanical systems do not allow predictions of their future state with arbitrary accuracy. For example, the outcome of a diffraction experiment such as the Davisson and Germer experiment can be predicted only in terms of a *probability distribution*. It is in possible to predict or calculate the *exact* trajectory of an individual quantum mechanical particle. The Heisenberg uncertainty principle (Heisenberg, 1927) allows us to *quantify the uncertainty associated with quantum mechanical particles*.

The uncertainty of a dynamical variable, $\Delta\xi$, is defined as

$$(\Delta\xi)^2 \; = \; \left\langle \left(\xi \; - \; \langle\xi\rangle\right)^2 \right\rangle . \tag{5.1}$$

Thus, $\Delta\xi$ is the *mean deviation* of a variable ξ from its expectation value $\langle\xi\rangle$. The *mean* deviation can be understood as the most probable deviation. Using the fact that the expectation value of a sum of variables is identical to the sum of the expectation values of these variables, that is

$$\left\langle \sum_i \xi_i \right\rangle \; = \; \sum_i \langle \xi_i \rangle \tag{5.2}$$

one obtains by squaring out Eq. (5.1)

$$(\Delta\xi)^2 \; = \; \left\langle \xi^2 \right\rangle \; - \; \langle\xi\rangle^2 . \tag{5.3}$$

Having *defined* the meaning of uncertainty, we proceed to *quantify* the uncertainty.

5.2 Position–momentum uncertainty

In order to quantify the uncertainty associated with a quantum mechanical system, consider a wave function of gaussian shape as shown in ***Fig***. 5.1. The position space wave function is given by the gaussian function

$$\psi(x) \quad = \quad \frac{A_x}{\sigma_x \sqrt{2\,\pi}} \; e^{-\frac{1}{2}\left(\frac{x}{\sigma_x}\right)^2} \; . \tag{5.4}$$

The constant A_x is used to normalize the wave function using $\langle\psi|\psi\rangle = 1$, which yields

$$A_x \quad = \quad (4\,\pi)^{1/4}\,\sqrt{\sigma_x}\; . \tag{5.5}$$

This wave function may represent a particle localized in a potential well. If the barriers of the well are sufficiently high the particle cannot escape from the well. That is, the wave function is stationary, *i. e*. $\psi(x)$ does not depend on time.

The momentum distribution which corresponds to the gaussian wave function can be obtained by the Fourier integral

$$\Phi(p) \quad = \quad \frac{1}{\sqrt{2\,\pi\,\hbar}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ipx/\hbar}\; dx. \tag{5.6}$$

Inserting the wave function, given by Eq. (5.4), into the Fourier integral yields

$$\Phi(p) \quad = \quad (4\,\pi)^{1/4} \sqrt{\frac{\hbar}{\sigma_x}} \; \frac{1}{\sqrt{2\,\pi}\;(\hbar/\sigma_x)} \; e^{-\frac{1}{2}\left(\frac{p}{\hbar/\sigma_x}\right)^2} \quad . \tag{5.7}$$

This function represents a gaussian function with a prefactor. Thus, the Fourier transform of a gaussian function is also a gaussian function. The gaussian function in Eq. (5.7) has a standard deviation of $\hbar / \sigma_x$ which has the dimension of momentum. Therefore, we introduce the standard deviation in momentum space

$$\sigma_p \quad = \quad \hbar\,/\,\sigma_x\; . \tag{5.8}$$

In analogy to Eq. (5.5), we define the normalization constant A_p as

$$A_p \quad = \quad (4\,\pi)^{1/4}\,\sqrt{\sigma_p}\quad . \tag{5.9}$$

Equation (5.7) can be rewritten using the normalization constant A_p.

$$\Phi(p) \quad = \quad \frac{A_p}{\sqrt{2\pi}\ \sigma_p}\ \mathrm{e}^{-\frac{1}{2}\left(\frac{p}{\sigma_p}\right)^2} \ . \tag{5.10}$$

This equation is formally identical to the position-space representation of the wave function given by Eq. (5.4). It can be easily verified that the momentum space representation of the state function is normalized as well $\langle \Phi(p) | \Phi(p) \rangle = 1$. The position and momentum representations of the wave function are shown in ***Fig***. 5.1.

The position space and momentum space representation of a gaussian wave function allows us to form the product of the position and momentum uncertainty using Eq. (5.8)

$$\sigma_x\ \sigma_p \quad = \quad \hbar \ . \tag{5.11}$$

Thus, the product of position uncertainty and momentum uncertainty is a constant. Hence a small position uncertainty results in a large momentum uncertainty and vice versa. The uncertainty of the position Δx, as defined by Eq. (5.1) is, in the case of a gaussian function, identical to the standard deviation σ_x of that gaussian function. Thus, Eq. (5.11) can be rewritten in its more popular form

$$\Delta x\ \Delta p \quad = \quad \hbar \ . \tag{5.12}$$

This relation was derived for gaussian wave functions and it applies, in a strict sense, only a gaussian wave functions. If the above calculation is performed for wave functions other than a gaussian (*e. g*. square-shaped or sinusoidal), then the uncertainty associated with Δx and Δp is larger. Hence, the general formulation of the ***position – momentum form of the Heisenberg uncertainty relation*** is given by

$$\boxed{\Delta x\ \Delta p \quad \geq \quad \hbar} \tag{5.13}$$

The uncertainty principle shows that an accurate determination of both, position and momentum, cannot be achieved. If a particle is localized on the x axis with a small position uncertainty Δx, then this localization is achieved at the expense of a large momentum uncertainty Δp.

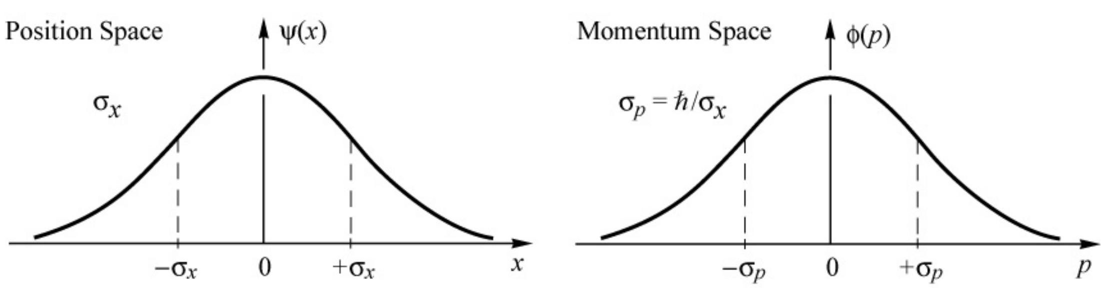

Fig. 5.1 Gaussian wave packet in position space (left). The momentum representation of the Gaussian wavepacket is also a gaussian function (right). The standard deviations are related by $\sigma_p = (h / 2\pi) / \sigma_x$. Thus a localized wave packet in position space results in a delocalized function in momentum space and vice versa.

5.3 Energy – time uncertainty

The uncertainty relation between position and momentum will now be modified using the group velocity relation, the de Broglie relation, and the Planck relation to obtain a second uncertainty relation between time and energy. The starting point for this modification is a wave packet that propagates with the group velocity $\nu_{gr} = \Delta x / \Delta t = \Delta\omega / \Delta k$. Inserting this relation and the de Broglie relation $\Delta p = \hbar \, \Delta k$ into the position-momentum uncertainty relation of Eq. (5.13) yields

$$\Delta t \, \Delta\omega \quad \geq \quad 1 . \tag{5.14}$$

It is now straightforward to obtain a second uncertainty relation by employing the Planck relation $\Delta E = \hbar \, \Delta\omega$, which yields

$$\boxed{\Delta E \, \Delta t \quad \geq \quad \hbar} \tag{5.15}$$

which is the ***energy – time form of the Heisenberg uncertainty relation***. This relation states that the energy of a quantum mechanical state can be obtained with highest precision (small ΔE), if the uncertainty in time is large, *i. e*. for transitions with a long lifetimes. The energetic width of quantum transitions given by the uncertainty principle is called the ***natural linewidth***.

The uncertainty relations are valid between the variables x and p (Eq. 5.13) as well as E and t (Eq. 5.15). These pairs of variables are called ***canonically conjugated variables***. A small uncertainty of one variable implies a large uncertainty of the other variable of the *same pair*. On the other hand, the two pairs of variables x, p and E, t are *independent*. For example a large uncertainty in the momentum does not allow any statement about the uncertainty in energy. The uncertainty principle requires that the deterministic nature of classical mechanics be revised. If an uncertainty of momentum or position exists, it is impossible to determine the future trajectory of a particle. On the other hand, the correspondence principle requires that quantum mechanics merges into classical mechanics in the classical limit. Therefore, the uncertainty of Δx or Δp should be insignificantly small in classical physics.

Exercise: ***Significance of the uncertainty principle in the macroscopic domain***. To see the insignificance of the uncertainty principle in the macroscopic physical world, a body with mass $m = 1$ kg and velocity $v = 1$ m / s is considered. The body moves along the x axis and the position of its centroid is assumed to be known to an accuracy of $\Delta x_0 = 1$ Å. Calculate the position uncertainty after a time of 10 000 seconds.

Solution: The initial momentum uncertainty is given by $\Delta p_0 \approx \hbar / \Delta x_0 \approx 10^{-24}$ kg m / s. After 10,000 seconds with no forces acting on the body, the position uncertainty is given by

$$\Delta x \quad = \quad \Delta x_0 \; + \; \frac{\Delta p_0}{m} t \quad \approx \quad 1 \text{ Å} \; + \; 10^{-10} \text{ Å} . \tag{5.16}$$

This exercise elucidates that the uncertainty principle does not contribute a significant uncertainty in classical mechanics. Thus, even though the trajectory of a macroscopic body cannot be determined in a strict sense, the associated uncertainty is insignificantly small. Even after a time of 10^{18} s (which is 30×10^9 years, *i. e*. approximately the age of the universe) the position uncertainty would be just 1 μm, which is still very small.
