Chapter 2: Elementary Aspects of Quantum Mechanics

→ We discuss some of the main concepts for the quantum mechanical description of <u>spin-less</u> and <u>non-relativistic particles</u> and the basics of the relevant mathematical background.

2.1. The Wave Function

→ A particle can be in (infinitely) many states. If the particle is in a <u>quantum mechanically unique state</u> we say that the particle is in a <u>pure state</u>.

<u>Classical mechanics:</u> A particle in a pure state at some time t is completely determined by quoting its position $\vec{x}$ and its velocity $\vec{v}$ at that time t. In a measurement of the position of the particle in this pure state, one will always (with 100% probability) obtain $\vec{x}$.

<u>Quantum mechanics:</u> A particle in a pure state at some time t is completely determined by quoting its <u>complex-valued wave function $\psi(\vec{x})$</u>, which satisfies the normalization condition

$$\int_{\mathbb{R}^3} d^3\vec{x}\, |\psi(\vec{x})|^2 = 1 .$$

States that probability to find the particle anywhere in $\mathbb{R}^3$ in a measurement of its position is unity.

The integral $\int_V d^3\vec{x}\, |\psi(\vec{x})|^2$ over an area $V \subset \mathbb{R}^3$ gives the probability to find the particle anywhere in the area V.

↳ $\rho(\vec{x}) := |\psi(\vec{x})|^2$: probability density for the location of the particle in a location measurement.

→ We can consider the wave function as a probability amplitude for a particle in the state $|\psi\rangle$ to end up in a pure state located at $\vec{x}$, $|\vec{x}\rangle$

↳ $\psi(\vec{x}) = \langle \vec{x} | \psi \rangle$ (→ There will be much more to this later...)

→ <u>Experimental realization:</u> probabilistic treatment using a large number N of equivalently prepared copies of the system being in state $|\psi\rangle$ (or: described by wave fct $\psi(\vec{x})$).

↳
- Detector D : signal if particle location happens to be in V → N_V counts
- Detector D' : signal if particle location happens to be in $V' = \mathbb{R}^3 \setminus V$ → $N_{V'}$ counts

↳ Exactly one of the detectors will always give a signal → $N_V + N_{V'} = N$

↳ In the limit $N \to \infty$ we find $\lim_{N\to\infty} \frac{N_V}{N} = \omega_V$ where $\omega_V = \int_V d^3\vec{x}\, |\psi(\vec{x})|^2$ (expectation value)

For finite N we have statistical fluctuations, and we find $\frac{N_V}{N}$ to be close to ω_V following the common statistical laws.

→ <u>Indeterministic aspect:</u> For a single copy one cannot predict whether D or D' will give a signal.
<u>Deterministic aspect:</u> One can give the probabilities for getting a signal from D and from D'.

→ Educational exercises:

(a) Realize the described measurement with $N < \infty$ copies. Calculate the probability p_n that detector D gives n counts ($n = 1, \dots, N$). Give mean value and standard deviation for n. → Hint: use binomial distribution

(b) Generalise discussion to the case of K subareas V_k ($\cup_{k=1}^{K} V_k = \mathbb{R}^3$) with detectors $D_1, \dots, D_K$.

2.2. The Position Measurement

← This section illustrates a number of formal aspects that will be made more concrete later.

→ The measurement of the position of the particle changes in general the state of the particle.

"Collapse of the state" (also: "Reduction of the wave packet"):

If detector D gives a signal, the particle is for sure (i.e. with 100% probability) in area V.
While the wave function of the particle was $\psi(\vec{x})$ before that measurement, it changes/collapses/reduces to the wave function

$$\tilde{\psi}(\vec{x}) = \frac{c_V(\vec{x})\,\psi(\vec{x})}{\sqrt{\int_V d^3x\,|\psi(\vec{x})|^2}}$$ after the measurement, where

$$c_V(\vec{x}) = \begin{cases} 1, & \vec{x} \in V \\ 0, & \vec{x} \notin V. \end{cases}$$

→ Linear operator: The operation "multiply wave function $\psi(\vec{x})$ with $c_V(\vec{x})$" is a linear operator acting on wave functions.

↳ An operator $\hat{O}$ acting on wave fcts is linear $\Leftrightarrow$ $\hat{O}(a_1\psi_1(\vec{x}) + a_2\psi_2(\vec{x})) = a_1\hat{O}(\psi_1(\vec{x})) + a_2\hat{O}(\psi_2(\vec{x}))$ for all wave fcts $\psi_i(\vec{x})$ and $a_{1,2} \in \mathbb{C}$

↳ Obviously true for $\hat{O}_V\psi(\vec{x}) := c_V(\vec{x})\psi(\vec{x})$.

→ Eigenfunctions:

↳ A wave fct $\phi(\vec{x})$ is called an eigenfunction of the linear operator $\hat{O}$ $\Leftrightarrow$ $\underbrace{\hat{O}\phi(\vec{x}) = \lambda\,\phi(\vec{x})}_{\text{eigenvalue equation}}$ for a $\lambda \in \mathbb{C}$ (eigenvalue)

The set of eigenvalues of a linear operator $\hat{O}$ is called the spectrum of $\hat{O}$.

↳ Eigenvalues for $\hat{O}_V\phi(\vec{x}) = c_V(\vec{x})\phi(\vec{x})$: $c_V(\vec{x})c_V(\vec{x}) = c_V(\vec{x})$ $\Rightarrow \lambda^2 = \lambda$ $\Rightarrow \lambda = 0, 1$, spectrum $= \{0, 1\}$
Eigenfunctions: $\lambda = 0$: all wave fcts for which $\phi(\vec{x}) = 0$ for all $\vec{x} \in V$
$\lambda = 1$: all wave fcts for which $\phi(\vec{x}) = 0$ for all $\vec{x} \notin V$
The operator represents the measurement "Is the particle in the area V?" which has the possible values yes (1) and no (0).
The corresponding normalized eigenfunctions are the wave functions for which the particle is to 100% inside the area V (1) and outside the area V (0), respectively.

→ Expectation value:

↳ The integral $\int_{\mathbb{R}^3} d^3x\, \psi^*(\vec{x})\,\hat{O}\,\psi(\vec{x})$ is called the expectation value of the linear operator $\hat{O}$ in the state described by the wave function $\psi(\vec{x})$. It gives the average of the measurement related to the operator $\hat{O}$.

↳ The expectation value of the operator "multiply wave function $\psi(\vec{x})$ with $c_V(\vec{x})$" gives the average of the measurement "Is the particle in the area V?", which is just $W_V = \int_{\mathbb{R}^3} d^3x\, \psi^*(\vec{x})\,c_V(\vec{x})\,\psi(\vec{x})$.

→ Location operator $\vec{X} = (X_1, X_2, X_3)$: linear multiplication operator $X_i \psi(\vec{x}) = x_i \psi(\vec{x})$, $i = 1,2,3$

↳ Eigenvalue equation $X_1 \phi(\vec{x}) = \bar{x}_1 \phi(\vec{x})$ has eigenvalues $\bar{x}_1 \in \mathbb{R}$ with eigenfcts $\phi(\vec{x}) = \delta(x_1 - \bar{x}_1) f(x_2, x_3)$ — arbitrary fct
The spectrum of X_1 is $\mathbb{R}$, and is continuous. The eigenfcts are distributions and cannot be normalized.

↳ Simultaneous eigenfcts for $\vec{X}$: $\phi_{\bar{\vec{x}}}(\vec{x}) = \delta(x_1 - \bar{x}_1)\delta(x_2 - \bar{x}_2)\delta(x_3 - \bar{x}_3) = \delta^{(3)}(\vec{x} - \bar{\vec{x}})$

$$\vec{X} \phi_{\bar{\vec{x}}}(\vec{x}) = \bar{\vec{x}} \phi_{\bar{\vec{x}}}(\vec{x})$$

The $\phi_{\bar{\vec{x}}}(\vec{x})$ are the limit (in the distribution sense) of a wave function that is more and more localized at location $\bar{\vec{x}}$.
The expectation value of $\vec{X}$ $\int_{\mathbb{R}^3} d^3\vec{x}\, \psi^*(\vec{x}) \vec{X} \psi(\vec{x}) = \int_{\mathbb{R}^3} d^3\vec{x}\, \vec{x} |\psi(\vec{x})|^2$ gives the average value of the position measurement for the state described by $\psi(\vec{x})$.
For N copies of the system in the state $\psi(\vec{x})$ we have $\sum_{k=1}^{N} \frac{\vec{x}(k)}{N} \xrightarrow{N\to\infty} \int_{\mathbb{R}^3} d^3\vec{x}\, \vec{x} |\psi(\vec{x})|^2$, where $\vec{x}(k)$ is the outcome for the location measurement for the k-th copy.

2.3. The Hilbert Space

→ The space of complex-valued and squared-integrable functions on $\mathbb{R}^3$

Can of course be defined in analogous way on $\mathbb{R}^n$ for any n.

$$L^2(\mathbb{R}^3) = \left\{ \psi : \mathbb{R}^3 \to \mathbb{C} \;\middle|\; \int_{\mathbb{R}^3} d^3\vec{x}\, |\psi(\vec{x})|^2 < \infty \right\}$$

defines an infinite-dimensional vector space over $\mathbb{C}$. $L^2(\mathbb{R}^3)$ is very useful for the quantum mechanical description of a particle in an "infinitely large box".
Those elements $\psi \in L^2(\mathbb{R}^3)$ for which $\int_{\mathbb{R}^3} d^3\vec{x}\, |\psi(\vec{x})|^2 = 1$ are the wave functions.

→ One can supplement the vector space $L^2(\mathbb{R}^3)$ with the concept of a (complex-valued) scalar product defined by

$$\langle \phi | \psi \rangle = \int_{\mathbb{R}^3} d^3\vec{x}\, \phi^*(\vec{x}) \psi(\vec{x}) \quad \text{with } \phi, \psi \in L^2(\mathbb{R}^3)$$

← Integral defined according to Lebesgue

which has the following properties:

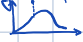
(S1) $\langle \phi | a_1\psi_1 + a_2\psi_2 \rangle = a_1 \langle \phi | \psi_1 \rangle + a_2 \langle \phi | \psi_2 \rangle$ for all $a_1, a_2 \in \mathbb{C}$, $\phi, \psi_1, \psi_2 \in L^2(\mathbb{R}^3)$
(S2) $\langle \phi | \psi \rangle = \langle \psi | \phi \rangle^*$ for all $\phi, \psi \in L^2(\mathbb{R}^3)$
(S3) $\langle \psi | \psi \rangle \geq 0$ and $\langle \psi | \psi \rangle = 0 \Leftrightarrow \psi = 0$ for all $\psi \in L^2(\mathbb{R}^3)$

} $\langle a_1\phi_1 + a_2\phi_2 | \psi \rangle = a_1^* \langle \phi_1 | \psi \rangle + a_2^* \langle \phi_2 | \psi \rangle$

→ Mathematically $L^2(\mathbb{R}^3)$ supplemented with the scalar product is a unitary vector space. The scalar product provides the notion of the "length" (norm) of an element of the vector space ("vector") and of an "angle" between two vectors.
$L^2(\mathbb{R}^3)$ has the property that it is complete with respect to the norm defined

$$\|\psi\| := \langle \psi | \psi \rangle^{1/2} \quad \text{for all } \psi \in L^2(\mathbb{R}^3).$$

Completeness means that each Cauchy sequence ψ_n $(n = 1, 2, \ldots, \infty)$ for $\psi_n \in L^2(\mathbb{R}^3)$ the limit for $n \to \infty$ is also contained inside $L^2(\mathbb{R}^3)$, i.e. $\lim_{n\to\infty} \psi_n = \psi \in L^2(\mathbb{R}^3)$. (Reminder Cauchy sequence: For every given real ε there is an integer N such that $\|\psi_m - \psi_n\| < \varepsilon$ for $m, n > N$.)

Second part of (S3): $\langle\psi|\psi\rangle = 0 \Rightarrow \psi = 0$ is guaranteed mathematically, if we identify all functions which differ only on a null set which does not contribute in integration. (example:  vs. )

Mathematically $L^2(\mathbb{R}^3)$ is an example for a **Hilbertspace**, which is an ∞-dimensional vector space over $\mathbb{C}$ with a scalar product $\langle\phi|\psi\rangle$ and with a norm $\|\psi\| := \langle\psi|\psi\rangle^{1/2}$ w.r.t. to which the vector space is complete.

2.4. Linear Operators

→ Let $\mathcal{H}$ be a Hilbert space (and we may have in mind $\mathcal{H} = L^2(\mathbb{R}^3)$).
The following mathematical considerations are essential for quantum mechanics.

→ **Linear operator:** An operator $A: \mathcal{H} \to \mathcal{H}$ that assigns each vector $\psi \in \mathcal{H}$ the vector $A\psi \in \mathcal{H}$ is a linear operator, if

$$A(c_1\psi_1 + c_2\psi_2) = c_1 A\psi_1 + c_2 A\psi_2 \quad \forall\, \psi_{1,2} \in \mathcal{H} \text{ and } c_{1,2} \in \mathbb{C}$$

→ **Adjoint operator:** The operator A^+ is called the adjoint operator to the linear operator A, if (and only if) aoi

$$\langle\phi|A^+\psi\rangle = \langle A\phi|\psi\rangle \quad \forall\, \phi,\psi \in \mathcal{H} \qquad A^+ \simeq \text{"A-dagger"}$$

↳ The following rules apply:
$$(aA + bB)^+ = a^* A^+ + b^* B^+$$
$$(AB)^+ = B^+ A^+$$
$$(A^+)^+ = A$$

→ **Hermitian (or self-adjoint) operator:** A linear operator A is called Hermitian, if aoi $A^+ = A$

↳ The operator $\mathcal{O}_V\psi = c_V(x)\psi$ from 2.2. is Hermitian.
The multiplication operator F: $(F\psi)(x) = f(x)\psi(x)$ is Hermitian in general as long as $f(x)\psi(x) \in L^2(\mathbb{R}^3)\ \forall \psi \in L^2(\mathbb{R}^3)$ and f is real-valued.

→ **Unitary operator:** A linear operator is called unitary if aoi $UU^+ = U^+U = \mathbb{1}$

→ **Eigenvalues and eigenvectors:** A $\psi \in \mathcal{H}$ is called eigenvector to the linear operator A with the eigenvalue a if aoi it has the property

$$A\psi = a\psi \quad \text{for an } a \in \mathbb{C}$$

↳ The set of eigenvalues of a linear operator A is called the **spectrum** of A.

↳ **Eigenvalues of Hermitian operators are real.**
Proof: $\langle\psi|A\psi\rangle = a\langle\psi|\psi\rangle = \langle A^+\psi|\psi\rangle = \langle A\psi|\psi\rangle = \langle\psi|A\psi\rangle^* = a^*\langle\psi|\psi\rangle \Rightarrow a = a^* \Rightarrow a \in \mathbb{R}$ ☒

↳ **The eigenvectors of a Hermitian operator to two different eigenvalues $a_1 \neq a_2$ are orthogonal.**
Proof: $A\psi_i = a_i\psi_i \Rightarrow \langle\psi_1|A\psi_2\rangle = \langle A\psi_1|\psi_2\rangle = a_1\langle\psi_1|\psi_2\rangle = a_2\langle\psi_1|\psi_2\rangle \Rightarrow (a_1 - a_2)\langle\psi_1|\psi_2\rangle = 0 \Rightarrow \langle\psi_1|\psi_2\rangle = 0$ ☒

→ **Orthonormal system (ONS):** A set of vectors $\phi_i \in \mathcal{H}$ $(i = 1, \dots, n)$ for which $\langle\phi_i|\phi_j\rangle = \delta_{ij}$ for all $i,j \in \{1,\dots,n\}$

→ **Completeness of $\mathcal{H}$:** Each vector $\psi \in \mathcal{H}$ can be written as a linear combination of a minimal set of basis vectors $\{\phi_1, \phi_2, \dots\}$, i.e. there is a unique set of complex numbers $\{c_1, c_2, \dots\}$, $c_n \in \mathbb{C}$ such that $\psi = \sum_n c_n \phi_n$; $c_n = \langle \phi_n | \psi \rangle$.

↳ If a Hermitian operator has several linear independent eigenvectors to the same eigenvalue ("degenerate eigenvalue") one can always construct an orthonormal basis to the set of eigenvectors to that eigenvalue.

→ **Spectral Theorem:** For each Hermitian operator A with a discrete spectrum there is a complete orthonormal basis to $\mathcal{H}$ made of eigenvectors $\{\phi_1, \phi_2, \dots\}$ to A, i.e. $A\phi_m = a_m \phi_m$ for some $a_m \in \mathbb{R}$.

Proof: → math lecture

$$A \sim \begin{pmatrix} a_1 & & & 0 \\ & a_2 & & \\ & & a_3 & \\ 0 & & & \ddots \end{pmatrix}$$

↳ The spectral theorem is a highly non-trivial statement which says that the (∞-dimensional) matrix associated to operator A can be made diagonal in a basis that consists of eigenvectors. For a general linear operator only a block-diagonal form can be achieved. →

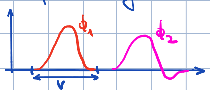
↳ Alternative naming: complete orthonormal system (CONS)

→ **Correspondence Principle:**
Each observable Quantity ("observable") in quantum mechanics is represented by a Hermitian operator.

→ The set of eigenvalues (spectrum) of the Hermitian operator associated to an observable in quantum mechanics is the set of measurable values of the observable.

→ **Projection operators:** A Hermitian operator ($\Pi^\dagger = \Pi$) which also satisfies $\Pi^2 = \Pi\Pi = \Pi$ is called a projection operator.

↳ The operator $O_V \psi = C_V(x)\psi$ from 2.2. (measurement: "Is the particle in area V (Yes/No)") is a projection operator. The spectrum of O_V is $\{0, 1\}$ and the sets of eigenvectors for both eigenvalues are both ∞-dimensional. Eigenvectors to eigenvalues 0 and 1 are mutually orthogonal



$C_V \phi_1 = \phi_1$, $C_V \phi_2 = 0$
$\langle \phi_1 | \phi_2 \rangle = 0$

→ **Completeness relation:** Let $\{\phi_1, \phi_2, \dots\}$ be a complete orthonormal system (CONS) of $\mathcal{H} = L^2(\mathbb{R}^3)$. We then have for any $\psi \in \mathcal{H}$:

$$\psi(\vec{x}) = \sum_n \phi_n(\vec{x}) \langle \phi_n | \psi \rangle = \sum_n \phi_n(\vec{x}) \int d^3\vec{y}\, \phi_n^*(\vec{y}) \psi(\vec{y}) = \int d^3\vec{y} \sum_n \phi_n(\vec{x}) \phi_n^*(\vec{y}) \psi(\vec{y}),$$

which we can write as

$$\sum_n \phi_n^*(\vec{x}) \phi_n(\vec{y}) = \delta^{(3)}(\vec{x} - \vec{y}) \quad \text{(completeness relation)}.$$

↳ The Dirac δ-function is not an element of $L^2(\mathbb{R}^3)$. It is not even a function, but a distribution, i.e. it is defined as a functional acting on the functions in $L^2(\mathbb{R}^3)$: $\mathcal{H} \to \mathbb{C}$ with $\int d^3\vec{x}\, \delta^{(3)}(\vec{x} - \vec{y}) \psi(\vec{x}) = \psi(\vec{y})$, $\psi \in L^2(\mathbb{R}^3)$.
However, it is possible to define it within $L^2(\mathbb{R}^3)$ through a sequence $\phi_n \in L^2(\mathbb{R}^3)$ ($n = 1, 2, \dots$) such that the functionals defined through the ϕ_n, $\int d^3\vec{x}\, \phi_n^*(\vec{x} - \vec{y}) \psi(\vec{x})$ have the property $\lim_{n\to\infty} \int d^3\vec{x}\, \phi_n^*(\vec{x} - \vec{y}) \psi(\vec{x}) = \psi(\vec{y})$.
Such a series can then be taken as a definition for the δ-function. The choice of the series ϕ_n does not need to be unique.
Example: $\phi_n(\vec{x}) = \left(\frac{n}{\pi}\right)^{3/2} \exp(-n\vec{x}^2)$, $n = 0, 1, 2, \dots$

↳ Note: $\int d^3\vec{x}\, \phi_n(\vec{x}) = 1$, but $\int d^3\vec{x}\, |\phi_n(\vec{x})|^2 = \left(\frac{n}{2\pi}\right)^{3/2} \to \infty$ for $n \to \infty$

03/07/2016 (5)

2.5. Scalar Product and Expectation Values

i.e. $\|\Psi\| = 1$

→ Consider a physical system in a pure state described by the state vector Ψ and an observable described by the Hermitian operator A which has a CONS of eigenvectors $\phi_1, \phi_2, \ldots$ with corresponding eigenvalues $a_1, a_2, \ldots$

some of the a_n can be equal

So we can "expand" Ψ in the ϕ_n (i.e. write as a linear combination of the ϕ_n) as

$$\Psi = \sum_n \phi_n \langle \phi_n | \Psi \rangle \qquad (*)$$

In this section we now discuss the probability to measure a certain value and the mean value obtained in a large number of measurements made on the state Ψ, applying the Hilbert space formalism.

→ If the eigenvalue a_n has exactly one eigenvector ("non-degenerate eigenvalue"), then the probability to obtain in a measurement of A the value a_n is $|\langle \phi_n | \Psi \rangle|^2$.

and we call the complex-valued $\langle \phi_n | \Psi \rangle$ the corresponding probability amplitude. The state Ψ is completely and uniquely characterized by the knowledge of the probability amplitudes $\langle \phi_n | \Psi \rangle$, see Eq. (*).

→ If some of the eigenvalues $a_1, a_2, \ldots$ are equal, e.g. $a_1 = a_2 =: a$ ("degenerate eigenvalue"), then the probability to obtain in a measurement of A the value a is

$$|\langle \phi_1 | \Psi \rangle|^2 + |\langle \phi_2 | \Psi \rangle|^2$$

→ The relation $\sum_n |\langle \phi_n | \Psi \rangle|^2 = \sum_n \langle \Psi | \phi_n \rangle \langle \phi_n | \Psi \rangle = \langle \Psi | \Psi \rangle = 1$ means that the probability of obtaining in a measurement any of the values $a_1, a_2, \ldots$ is unity, which is directly connected to the norm of the state vector being unity.

→ The average of the measured values of the observable A (with a discrete spectrum) is given by

$$\sum_n a_n |\langle \phi_n | \Psi \rangle|^2 = \sum_n a_n \langle \Psi | \phi_n \rangle \langle \phi_n | \Psi \rangle = \sum_n \langle \Psi | \phi_n \rangle \langle a_n \phi_n | \Psi \rangle = \sum_n \langle \Psi | \phi_n \rangle \langle A \phi_n | \Psi \rangle$$
$$= \sum_n \langle \Psi | \phi_n \rangle \langle \phi_n | A \Psi \rangle = \langle \Psi | \sum_n \phi_n \langle \phi_n | A \Psi \rangle \rangle = \langle \Psi | A \Psi \rangle$$

and is called the expectation value of the observable A.

→ For the case of an observable operator with a continuous spectrum there are some modifications.

Example: Location operator in 1 dimension $\quad X \Psi(x) = x \Psi(x)$

↳ Eigenfunctions: $\phi_y(x) = \delta(x-y)$, $\quad X \phi_y(x) = y \phi_y(x)$ for all $x \in \mathbb{R}$

Problem: ϕ_y are not normalizable since they are distributions and thus not directly contained in $L^2(\mathbb{R})$

However: they are orthogonal in the sense $\langle \phi_y | \phi_{y'} \rangle = \int_{-\infty}^{+\infty} dx \, \phi_y^*(x) \phi_{y'}(x) = \int dx \, \delta(x-y) \delta(x-y') = \delta(y-y')$

and they form a complete orthogonal basis because each function $\Psi(x) \in L^2(\mathbb{R})$ can be written as a linear combination of the ϕ_y

$$\Psi(x) = \int_{-\infty}^{+\infty} dy \, \delta(x-y) \Psi(y) = \int_{-\infty}^{+\infty} dy \, \phi_y(x) \Psi(y)$$

where

$$\Psi(y) = \langle \phi_y | \Psi \rangle = \int_{-\infty}^{+\infty} dx \, \phi_y^*(x) \Psi(x) = \int_{-\infty}^{+\infty} dx \, \delta(x-y) \Psi(x)$$

→ It is very convenient to write $\langle x|\psi\rangle := \langle\phi_x|\psi\rangle$, so that $\psi(x) = \langle x|\psi\rangle$.
We see that $|\psi(x)|^2 = |\langle x|\psi\rangle|^2$ is the location probability density of the state (continuous spectrum), so $|\langle x|\psi\rangle|^2 dx = |\psi(x)|^2 dx$ is the probability to measure the location of the system (e.g. particle) in the intervall $[x, x+dx]$. We usually interpret this as the intervall in which the particle is observed.
The average location of the particle is the expectation value $\langle\psi|X\psi\rangle = \int_{-\infty}^{+\infty} dx\, x\, |\psi(x)|^2 = \int_{-\infty}^{+\infty} dx\, \psi^*(x)\, x\, \psi(x)$

→ From a mathematical point of view X is an example for an unbounded operator, which means that there are $\psi \in L^2(\mathbb{R})$ for which $X\psi \notin L^2(\mathbb{R})$.

→ Formally one calls an operator $A: \mathcal{H} \to \mathcal{H}$ a bounded operator if there is a real $C \geq 0$, such that $\|A\psi\| \leq C\|\psi\|$ for all $\psi \in \mathcal{H}$. One can then define the norm of the operator A as

$$\|A\| := \sup_{\substack{\psi\in\mathcal{H} \\ \|\psi\|=1}} \|A\psi\|$$ which is finite.

→ Mathematically, the issue of an operator being unbounded is directly connected with its spectrum containing a continuous interval of eigenvalues, which is yet directly connected that δ-functions are involved for the eigenfunctions. In analogy to the δ-function, which one can define (indirectly) within $L^2(\mathbb{R})$ using the concepts of "sequence" and functional one can also generalize the concepts of Hermitian bounded operators (for which we learn most of the mathematical rules in introductory quantum physics courses) to Hermitian unbounded operators (such as the X and P operators, which we actually use in quantum physics most of the time).

This formalism is quite involved but turns out to be of little practical use in actual applications of quantum mechanics because the outcome is that the basic calculational rules for bounded and unbounded operators are essentially the same once one deals with δ-functions like regular functions, generalizes sums to integrals and considers the existence of infinite dimensional and/or continuous matrices.
We will therefore not mathematically dwell on unbounded operators any deeper.

↳ See literature: John v. Neumann: Mathematical Foundation of Quantum Mechanics ← !
Walter Tirring: Lehrbuch der Mathematischen Physik, Bd. 3 Quantenmechanik

→ Educational exercises:
(a) Show that an operator which has a spectrum containing a continuous intervall is indeed unbounded.
(b) One can generalize the concept of the "spectrum" from bounded to unbounded operators by defining the spectrum of an operator A by the set of values $z \in \mathbb{C}$ for which the operator $R_A(z) = \frac{1}{z-A}$ is unbounded.
Show that the spectrum of X is indeed $\mathbb{R}$.
(c) Show that the spectrum of the momentum operator P is $\mathbb{R}$.

2.6. The Momentum

→ From classical mechanics we know that there is a connection between spatial translations and the momentum of a physical system. We use this connection to motivate the form of the momentum operator in quantum mechanics.

↳ We consider a 1-dimensional system for simplicity most of the time, with obvious generalizations to 3 dimensions.

→ Translation operator T_a: T_a shift a wave function by distance a, so

$$(T_a \psi)(x) = \psi(x-a).$$

↳ We have: $T_a T_b = T_b T_a = T_{a+b}$, $T_\emptyset = \mathbb{1}$, $T_a^+ = T_{-a}$ (exercise!) $\Rightarrow T_a T_a^+ = T_a^+ T_a = \mathbb{1}$
so T_a is a unitary (but not a Hermitian) operator.

↳ Infinitesimal translation: $T_a \psi(x) = \psi(x-a) \overset{a \ll 1}{\approx} \psi(x) - a\frac{d}{dx}\psi(x) = (\mathbb{1} - \frac{ia}{\hbar} \underbrace{\frac{\hbar}{i}\frac{\partial}{\partial x}}_{=: P \text{ operator}})\psi(x)$

↳ We apply the P-operator to a de Broglie wave:

$$P \exp\left[\frac{i}{\hbar}(px - Et)\right] = \frac{\hbar}{i}\frac{\partial}{\partial x}\exp\left[\frac{i}{\hbar}(px-Et)\right] = \underset{\text{momentum!}}{p}\exp\left[\frac{i}{\hbar}(px-Et)\right]$$

which should be an eigenfunction of the momentum operator.

↳ P is a Hermitian operator: We use that $\phi \in L^2(\mathbb{R})$ fall of sufficiently fast at $\pm\infty$ and integration by parts.

$$\int_{-\infty}^{+\infty} dx\, \phi^*(x) \frac{\hbar}{i}\frac{d}{dx}\phi(x) = -\int dx \left(\frac{\hbar}{i}\frac{d}{dx}\phi^*(x)\right)\phi(x) = \int dx\left(\frac{\hbar}{i}\frac{d}{dx}\phi(x)\right)^* \phi(x) \quad ✓$$

→ The quantum mechanical operator representing the measurement of the momentum $\vec{p}$ of a system is

$$\vec{P} = \frac{\hbar}{i}\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) = \frac{\hbar}{i}\frac{\partial}{\partial \vec{x}}$$

↳ Eigenfunctions and eigenvalues: $P f(x) = \frac{\hbar}{i}\frac{d}{dx}f(x) = p f(x)$ with $p \in \mathbb{R}$

gives the unique solution $f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$

↳ The momentum operator is unbounded, its spectrum is continuous and its eigenfunctions f_p cannot be normalized, but the f_p are orthogonal to each other in the sense that

$$\langle f_p | f_{p'} \rangle = \int_{-\infty}^{+\infty} dx\, f_p^*(x) f_{p'}(x) = \int_{-\infty}^{+\infty} \frac{dx}{2\pi\hbar} e^{-ipx/\hbar} e^{ip'x/\hbar} = \int_{-\infty}^{+\infty} \frac{d\bar{x}}{2\pi} e^{-i(p-p')\bar{x}} = \delta(p-p').$$

This is in analogy to the eigenfunctions of the location operator X.

↳ We use the Fourier transformation formalism to write the wave function $\psi(x)$ as a superposition (which is the continuous generalization of the notion of linear combination) of the $f_p(x)$:

$$\psi(x) = \int_{-\infty}^{+\infty} dp\, f_p(x)\, \tilde{\psi}(p) = \int_{-\infty}^{+\infty} dp \frac{e^{ipx/\hbar}}{(2\pi\hbar)^{1/2}}\tilde{\psi}(p)$$

because of $\langle f_p | f_{p'} \rangle = \delta(p-p')$ we have

$$\tilde{\psi}(p) = \langle f_p | \psi \rangle = \int_{-\infty}^{+\infty} dx \frac{e^{-ipx/\hbar}}{(2\pi\hbar)^{1/2}} \psi(x) \quad \text{which we from now write as} \quad \tilde{\psi}(p) = \langle p | \psi \rangle$$

↳ We see: $\tilde{\psi}(p) = \langle f_p | \psi \rangle$ is the probability amplitude for measuring the momentum p in the state ψ:

$|\tilde{\psi}(p)|^2$: probability density for the momentum of the particle / system in a momentum measurement

$|\tilde{\psi}(p)|^2 dp$: probability to measure a momentum in the intervall $[p, p+dp]$ in a momentum measurement

↳ We call $\tilde{\psi}(p) = \langle p | \psi \rangle$ the <u>momentum space wave function</u> or <u>momentum space probability amplitude</u>.

↳ The knowledge of $\langle p | \psi \rangle = \tilde{\psi}(p)$ is physically equivalent to the knowledge of $\langle x | \psi \rangle = \psi(x)$. So we can interpret using $\langle p | \psi \rangle$ vs. $\langle x | \psi \rangle$ simply as different representations of the same state ψ, in the sense that we either use a momentum state basis or a configuration space basis.

↳ We can even go one step further and consider $|\psi\rangle, |x\rangle, |p\rangle$ as well as operators as abstract objects that do exist independent of the choice of representation.

→ <u>Configuration space and momentum space representations:</u>

$$\psi(x) = \langle x | \psi \rangle = \int_{-\infty}^{+\infty} dp \underbrace{\langle x | p \rangle}_{\frac{1}{(2\pi\hbar)^{1/2}} e^{ipx/\hbar}} \underbrace{\langle p | \psi \rangle}_{\tilde{\psi}(p)} \qquad \tilde{\psi}(p) = \langle p | \psi \rangle = \int_{-\infty}^{+\infty} dx \underbrace{\langle p | x \rangle}_{\frac{1}{(2\pi\hbar)^{1/2}} e^{-ipx/\hbar}} \underbrace{\langle x | \psi \rangle}_{\psi(x)}.$$

$$\Rightarrow \int_{-\infty}^{+\infty} dx\, |x\rangle\langle x| = \int_{-\infty}^{+\infty} dp\, |p\rangle\langle p| = \mathbb{1} \qquad \text{(generalized completeness relation for } p \text{ and } x \text{ eigenstates)}$$

$$\langle \phi | \psi \rangle = \int_{-\infty}^{+\infty} dx \underbrace{\langle \phi | x \rangle}_{\phi^*(x)} \underbrace{\langle x | \psi \rangle}_{\psi(x)} = \int_{-\infty}^{+\infty} dp \underbrace{\langle \phi | p \rangle}_{\tilde{\phi}^*(p)} \underbrace{\langle p | \psi \rangle}_{\tilde{\psi}(p)} \qquad \text{(scalar product)}$$

This is the abstract representation-free momentum operator.

↳ We see: $\langle p | P \psi \rangle = \int dp' \langle p | P | p' \rangle \langle p' | \psi \rangle = \int dp' \, p' \, \delta(p-p') \tilde{\psi}(p) = p \, \tilde{\psi}(p)$

$= \langle p | P \psi \rangle = \langle P p | \psi \rangle = p \langle p | \psi \rangle = p \, \tilde{\psi}(p)$

so the momentum operator P is a simple multiplication operator in momentum space.

$$\langle x | P | \psi \rangle = \int dp' \, p' \langle x | p' \rangle \langle p' | \psi \rangle = \int \frac{dp'}{(2\pi\hbar)^{1/2}} p' e^{ip'x/\hbar} \tilde{\psi}(p') = \frac{\hbar}{i} \frac{d}{dx} \int \frac{dp'}{(2\pi\hbar)^{1/2}} e^{ip'x/\hbar} \tilde{\psi}(p') = \frac{\hbar}{i} \frac{d}{dx} \psi(x)$$

$$\langle x | X | \psi \rangle = x \langle x | \psi \rangle = x \, \psi(x)$$

X operator in momentum space

$$\langle p | X | \psi \rangle = \int dx' \, x' \langle p | x' \rangle \langle x' | \psi \rangle = \int \frac{dx'}{(2\pi\hbar)^{1/2}} x' e^{-ipx'/\hbar} \psi(x') = i\hbar \frac{d}{dp} \tilde{\psi}(p)$$

03/07/2016 (9)

→ **Commutation relation of X and P operators:** $\boxed{[X,P] := XP - PX = i\hbar \mathbb{1}}$

↳ check in x-space: $\left(x \frac{\hbar}{i}\frac{d}{dx} - \frac{\hbar}{i}\frac{d}{dx} x\right)\psi(x) = \cancel{x\frac{\hbar}{i}\psi'(x)} - \frac{\hbar}{i}\psi(x) - \cancel{\frac{\hbar}{i}x\psi'(x)} = i\hbar\,\psi(x)$ for all $\psi(x)$ ✓

check in p-space: $\left(i\hbar\frac{d}{dp}p - p\,i\hbar\frac{d}{dp}\right)\tilde{\psi}(p) = i\hbar\,\tilde{\psi}(p) + \cancel{i\hbar p\tilde{\psi}'(p)} - \cancel{p\,i\hbar\tilde{\psi}'(p)} = i\hbar\,\tilde{\psi}(p)$ for all $\tilde{\psi}(p)$ ✓

→ Generalization to 3 spatial dimensions:

$$\psi(\vec{x}-\vec{a}) = \psi(\vec{x}) - \vec{a}\vec{\nabla}\psi(\vec{x}) = \psi(\vec{x}) - \frac{i\vec{a}}{\hbar}\frac{\hbar}{i}\vec{\nabla}\psi(\vec{x})$$

$$\vec{P} = -i\hbar\vec{\nabla} = -i\hbar\frac{\partial}{\partial\vec{x}}$$

$$\vec{P} f_{\vec{p}}(\vec{x}) = \vec{p} f_{\vec{p}}(\vec{x}) \quad \text{with} \quad f_{\vec{p}}(\vec{x}) = \langle\vec{x}|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\vec{x}/\hbar} = \langle\vec{x}|\vec{p}\rangle$$

$$\langle f_{\vec{p}}|f_{\vec{p}'}\rangle = \langle\vec{p}|\vec{p}'\rangle = \delta^{(3)}(\vec{p}-\vec{p}') = \delta(p_x-p_x')\,\delta(p_y-p_y')\,\delta(p_z-p_z')$$

$$\int d^3\vec{x}\, |\vec{x}\rangle\langle\vec{x}| = \int d^3\vec{p}\, |\vec{p}\rangle\langle\vec{p}| = \mathbb{1}$$

$$\psi(\vec{x}) = \langle\vec{x}|\psi\rangle = \int d^3\vec{p}\, \langle\vec{x}|\vec{p}\rangle\langle\vec{p}|\psi\rangle$$

$$\tilde{\psi}(\vec{p}) = \langle\vec{p}|\psi\rangle = \int d^3\vec{x}\, \langle\vec{p}|\vec{x}\rangle\langle\vec{x}|\psi\rangle$$

$$[X_k, P_l] = i\hbar\,\delta_{kl}\,\mathbb{1}, \quad k,l = 1,2,3$$

→ X and P operators from different spatial directions commute!