

2.7. Dirac Notation

→ We have seen that spatial wave function $\psi(x) = \langle \hat{x} | \psi \rangle$, momentum space wave function $\tilde{\psi}(p) = \langle \hat{p} | \psi \rangle$ and the set of scalar products $\{\langle \phi_1 | \psi \rangle, \langle \phi_2 | \psi \rangle, \dots\}$ with respect to a CONS $\{\phi_1, \phi_2, \dots\}$ carry the complete information on the quantum state ψ and that they should be considered as coordinates of the quantum state w.r.t. to different bases.

→ P.A.M. Dirac: Formalism for "abstract" and basis-independent state vectors.

& Generalisation of the Hilbert space \mathcal{H} to contain the abstract state vectors.

↳ "ket-vector" $| \psi \rangle \in \mathcal{H}$
 "bra-vector" $\langle \psi | \in \text{Dual space } (\mathcal{H})$ → $\begin{cases} \langle \psi | \text{ is the dual space vector to } | \psi \rangle \\ \text{analogy: } \hat{a} = \left(\begin{smallmatrix} 0 & \psi \\ 0 & 0 \end{smallmatrix} \right) \Leftrightarrow | \psi \rangle \text{ and } \hat{a}^+ = (a_1^*, a_2^*, \dots) \Leftrightarrow \langle \psi | \end{cases}$
 but meant abstract and not w.r.t. to specific basis
 Scalar product: $\langle \phi_i | \psi \rangle$ product of a bra and a ket-vector ("bra-ket")

$\langle \phi_i | \psi \rangle$ are the complex coefficients / projections of state vector $| \psi \rangle$ on the CONS $\{ | \phi_i \rangle \}$

→ Let us use abbreviated notation $| n \rangle = | \phi_n \rangle$. In Dirac notation we have:

$$| \psi \rangle = \sum_n | n \rangle \langle n | \psi \rangle \quad \text{"decomposition of state } | \psi \rangle \text{ in basis vectors } | n \rangle \text{"}$$

$$\langle n | m \rangle = \delta_{nm} \quad \text{"orthogonality relation"}$$

$$\sum_n | n \rangle \langle n | = \mathbb{1} \quad \text{"completeness relation"} \quad \mathbb{1} : \text{abstract identity operator}$$

→ Let $\{ | n \rangle \}$ be the CONS of eigenvectors of the Hermitian operator A with eigenvalues a_n , then we can write

$$\begin{aligned} A &= \sum_n a_n | n \rangle \langle n | && \text{"spectral representation"} \\ \hookrightarrow f(A) &= \sum_n f(a_n) | n \rangle \langle n | && \text{"function of } A \text{"} \end{aligned} \quad \left. \begin{array}{l} \text{Abstract + representation} \\ \text{independent form of the} \\ \text{operator } A ! \end{array} \right\}$$

obvious generalization
to 3 spatial dimensions

→ The spatial wave function $\psi(x)$ is the projection of the state vector $| \psi \rangle$ on the continuous basis (functional) states $| x \rangle$ of the location operator X . We can write

$$\begin{aligned} X | x \rangle &= x | x \rangle, \quad \langle x | y \rangle = \delta(x-y), \quad \int_{-\infty}^{+\infty} dx | x \rangle \langle x | = \mathbb{1} \\ X &= \int_{-\infty}^{+\infty} dx x | x \rangle \langle x |, \quad f(X) = \int_{-\infty}^{+\infty} dx f(x) | x \rangle \langle x | \end{aligned} \quad \begin{array}{l} \text{"State } | \psi \rangle \text{ in configuration space"} \\ \text{"representation"} \end{array}$$

→ The momentum space wave function $\tilde{\psi}(p)$ is the projection of the state vector $| \psi \rangle$ on the continuous basis (functional) states $| p \rangle$ of the momentum operator P . We can write

$$\begin{aligned} P | p \rangle &= p | p \rangle, \quad \langle p | q \rangle = \delta(p-q), \quad \int_{-\infty}^{+\infty} dp | p \rangle \langle p | = \mathbb{1} \\ P &= \int_{-\infty}^{+\infty} dp p | p \rangle \langle p |, \quad f(P) = \int_{-\infty}^{+\infty} dp f(p) | p \rangle \langle p | \\ \langle x | p \rangle &= \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \end{aligned} \quad \begin{array}{l} \text{"State } | \psi \rangle \text{ in momentum space"} \\ \text{"representation"} \end{array}$$

← gives connection between momentum and configuration space representation

2.8. Uncertainty Relation

→ Let us consider a system in pure state $|4\rangle$ and observable (associated to operator) A.

The expectation value (of measurements) of A (on many copies of the system in state $|4\rangle$) is $\langle A \rangle = \langle 4 | A | 4 \rangle$.
The variance (of these measurements) is

$$\langle \Delta A \rangle^2 := \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2$$

The standard deviation is $\Delta A = \sqrt{\langle (A - \langle A \rangle)^2 \rangle} = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$

Note: * The variance and standard deviations just discussed are not related to any imprecision in the measurement but a property of the quantum nature of the state $|4\rangle$.

* $\Delta A = 0$ is possible if the system is in an eigenstate of A.

→ Now consider the measurement of two observables A and B, i.e. one makes measurements of A on many copies of the system in state $|4\rangle$ and the same for observable B.

Question: Can we make any general statements on the relation between ΔA and ΔB (if any)?

→ For any (not necessarily Hermitian) operator C we have: $\langle C^\dagger C \rangle = \langle 4 | C^\dagger C | 4 \rangle = \langle C | C | 4 \rangle \geq 0$

Let A, B be Hermitian. We define the non-Hermitian operator $C = \frac{A - \langle A \rangle}{\Delta A} + i \frac{B - \langle B \rangle}{\Delta B}$

$$\begin{aligned} \Rightarrow \langle C^\dagger C \rangle &= \left\langle \left(\frac{A - \langle A \rangle}{\Delta A} + i \frac{B - \langle B \rangle}{\Delta B} \right)^\dagger \left(\frac{A - \langle A \rangle}{\Delta A} + i \frac{B - \langle B \rangle}{\Delta B} \right) \right\rangle \\ &= \left\langle \left(\frac{A - \langle A \rangle}{\Delta A} - i \frac{B - \langle B \rangle}{\Delta B} \right) \left(\frac{A - \langle A \rangle}{\Delta A} + i \frac{B - \langle B \rangle}{\Delta B} \right) \right\rangle \\ &= \frac{(\Delta A)^2}{(\Delta A)^2} + \frac{(\Delta B)^2}{(\Delta B)^2} + \frac{1}{\Delta A \Delta B} \langle AB - BA \rangle = 2 + \frac{1}{\Delta A \Delta B} \langle AB - BA \rangle \geq 0 \end{aligned}$$

This is a real number!

So $[A, B]$ is always purely imaginary
unless $[A, B] = 0$

$$\Rightarrow \Delta A \Delta B \geq -\frac{1}{2} \langle [A, B] \rangle$$

$$\text{For } \langle CC^\dagger \rangle \text{ we obtain } \Delta A \Delta B \geq +\frac{1}{2} \langle [A, B] \rangle$$

→ General uncertainty relation: $\Delta A \Delta B \geq \frac{1}{2} |i \langle [A, B] \rangle|$

→ The uncertainty relation is a direct consequence of the postulates of quantum mechanics:

- (a) state described by wave function
- (b) correspondence principle: observable \leftrightarrow Hermit. operators
- (c) probability postulates for measurements

Examples:

→ Uncertainty relation for location and momentum measurements :

$$\hookrightarrow [X, P] = i\hbar \mathbb{I} \quad \leftarrow \text{unit operator!}$$

$$\hookrightarrow \boxed{\text{Heisenberg's Uncertainty Relation : } \Delta X \Delta P \geq \frac{\hbar}{2}}$$

↳ Applies for measurements on (many copies of) a system in a (same, unique) pure quantum state.
Which quantum state that is, does not matter, because $[X, P]$ is proportional to the unit operator.

↳ Note that Heisenberg's uncertainty relation does not mean that one cannot make arbitrarily precise location and momentum measurements.
It means that there is no state for which (measurements on many copies of the system in that system give) $\Delta X \Delta P < \frac{\hbar}{2}$.

↳ Heisenberg's uncertainty principle does not mean that a measurement of the location affects the momentum of the particle.
It is about measurements of either location or momentum made independently on many identical copies of the particle.

↳ It is well possible to prepare a state ($\psi(x) \rightarrow \delta(x-x_0)$) for which $\Delta X \rightarrow 0$, but for that state also $\Delta P \rightarrow \infty$, so that $\Delta X \Delta P$ always $\geq \frac{\hbar}{2}$.

→ Observables A and B commute: $[A, B] = 0 \Rightarrow \Delta A \Delta B \geq 0$

Case (a): $\Delta A \Delta B = 0$ if the state of the system is eigenstate of A or B (or both)

Case (b): $\Delta A \Delta B > 0$ if state of the system is neither eigenstate of A nor of B.

↳ Note that $\Delta A \Delta B$ can become very large depending on the spectrum of A and B and on the state.

→ Construction of the state for which $\Delta X \Delta P = \frac{\hbar}{2}$:

↳ In the general calculation above we get "=" signs if $\langle C | C^\dagger | C \rangle = \langle C | C | C \rangle = 0 \Leftrightarrow |C\rangle = 0$

$$\Leftrightarrow |C\rangle = 0 \text{ for } C = \frac{X-x_0}{\epsilon} + i \frac{P-P_0}{\hbar \sqrt{2}} \quad (\Delta X = \epsilon, \Delta P = \frac{\hbar}{2\epsilon} \text{ so that } \Delta X \Delta P = \frac{\hbar}{2})$$

$$\Leftrightarrow (\text{config space}) \quad \left[\frac{X-x_0}{\epsilon} + \frac{2i\epsilon}{\hbar} \left(\frac{\hbar}{i} \frac{d}{dx} - P_0 \right) \right] \psi(x) = 0$$

$$\text{This gives : } \psi(x) = N \exp\left(-\frac{(x-x_0)^2}{4\epsilon^2}\right) e^{-iP_0 x \over \hbar}$$

2.9. Time Evolution and Schrödinger Equation

→ Up to now we did not consider the time evolution of wave functions, but we already discussed the de Broglie wave function $\exp\left[\frac{i}{\hbar}(p\vec{x} - E(p)t)\right]$ with $p = \hbar k$, $E(p) = \frac{p^2}{2m} + \hbar \omega$ that describes a free non-relativistic particle with a sharp momentum \vec{p} as a function of time. ("free monochromatic wave").

↪ Not normalizable

→ Construction of a normalizable wave function through a superposition of de Broglie wave functions: (1 dimension)

$$\Psi(x,t) = \int_{-\infty}^{+\infty} dp \frac{e^{ipx}}{\sqrt{2\pi\hbar}} e^{-i\frac{p^2}{2m}\frac{t}{\hbar}} \tilde{\Psi}(p) = \tilde{\Psi}(p,t)$$

$\tilde{\Psi}(p,t)$: momentum space time-dependent wave function
 $\hookrightarrow |\tilde{\Psi}(p,t)|^2 = |\tilde{\Psi}(p)|^2$: momentum distribution time-independent!

→ $\tilde{\Psi}(p,t)$ satisfies the Schrödinger equation for a free particle in momentum space:

$$i\hbar \frac{\partial}{\partial t} \tilde{\Psi}(p,t) = \frac{p^2}{2m} \tilde{\Psi}(p,t)$$

$\Psi(x,t)$ satisfies the corresponding Schrödinger equation in configuration space:

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = \frac{1}{2m} \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right)^2 \Psi(x,t)$$

→ The Hermitian operator corresponding to the observable "Energy of the particle/system" is called Hamilton operator H .

↪ $H_{\text{free particle}} = \frac{p^2}{2m}$ mom space: $\frac{p^2}{2m}$ config space: $-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$ (1 dim)

$H_{\text{free particle}} = \frac{\vec{p}^2}{2m}$ $\frac{p^2}{2m}$ $-\frac{\hbar^2}{2m} \vec{\nabla}^2$ (3 dim)

→ The Schrödinger equation gives the time-evolution of the state of a system.

The representation-independent, abstract version has the form

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H |\Psi(t)\rangle$$

and the solution for the time-evolution reads $|\Psi(t)\rangle = e^{-iHt/\hbar} |\Psi(0)\rangle$

↪ The Schrödinger equation describes the time-evolution while the system is left alone, without any external disturbance or any measurement.

↪ The unitary operator $\exp(-i\frac{Ht}{\hbar})$ is called time evolution operator.

→ Computation of the time-dependent configuration space wavefunction for a free particle: (1 dim.)

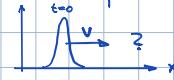
$$\begin{aligned}\psi(x,t) &= \langle x | \psi(t) \rangle = \langle x | e^{-iHt/\hbar} |\psi(0)\rangle \quad \leftarrow \text{insert } 1 = \int_{-\infty}^{+\infty} dp |p\rangle \langle p| \\ &= \int_{-\infty}^{+\infty} dp \langle x | e^{-iHt/\hbar} |p\rangle \langle p | \psi(0) \rangle \quad \leftarrow \text{use } H = \frac{p^2}{2m} \rightarrow H |p\rangle = \frac{p^2}{2m} |p\rangle, \\ &= \int_{-\infty}^{+\infty} dp \langle x | p \rangle \langle p | \psi(0) \rangle = e^{-\frac{i p x}{2m}} \langle p | \psi(0) \rangle \\ &= \int_{-\infty}^{+\infty} \frac{dp}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}} e^{-\frac{i p^2 t}{2m\hbar}} \psi(p)\end{aligned}$$

↳ We can determine the overall time-evolution of the wave function from its expansion in a CONS of states that are eigenstates of the energy operator, which is just the Hamilton operator.

↳ In the case of a free particle the energy eigenstates are just the $|p\rangle$ eigenstates because $E = \frac{p^2}{2m}$.

→ Example: Gaussian wave packet → Concrete realization for a particle wave with a realistic spatial shape that moves with momentum p_0 .

↳ Question: How does the shape of the wave packet evolve with time?



$$\psi(x, t=0) = \frac{1}{(2\pi)^{1/4} \sigma^{1/2}} e^{-\frac{x^2}{4\sigma^2}} \underbrace{e^{-\frac{ip_0 x}{\hbar}}} \underbrace{\text{drives the motion with } v = \frac{p_0}{m}}_{\text{Config wave function at } t=0}$$

$$\psi(p, t=0) = \frac{1}{(2\pi)^{1/4} (\Delta p)^{1/2}} e^{-\frac{(p-p_0)^2}{4(\Delta p)^2}}, \quad \Delta p = \frac{\hbar}{2\sigma} \quad \text{momentum space wave function}$$

) exercises

Gaussian centered at p_0 with the width Δp

$$\begin{aligned}\Rightarrow \psi(x, t) &= \int_{-\infty}^{+\infty} \frac{dp}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}} \langle p | \psi(0) \rangle = \int_{-\infty}^{+\infty} \frac{1}{(2\pi)^{1/4} (\Delta p)^{1/2}} e^{-\frac{(p-p_0)^2}{4(\Delta p)^2}} \\ &= \frac{1}{(2\pi)^{1/4} (\sigma + i \Delta p t/m)^{1/2}} \exp\left(-\frac{i p_0 t}{2\sigma t}\right) \exp\left(\frac{ip_0 x}{\hbar}\right) \exp\left(-\frac{(x-p_0 t/m)^2}{4(\sigma^2 + (\Delta p t/m)^2)}\right)\end{aligned}$$

) exercises

$$\Rightarrow |\psi(x, t)|^2 = \frac{1}{(2\pi)^{1/2}} \frac{\exp\left(-\frac{(x-p_0 t/m)^2}{2(\sigma^2 + (\Delta p t/m)^2)}\right)}{\left(\sigma^2 + \left(\frac{\Delta p t}{m}\right)^2\right)^{1/2}}$$



↳ We observe the following generic features:

* Maximum moves with $x^{max}(t) = \frac{p_0 t}{m}$, i.e. with velocity $v = \frac{p_0}{m}$

* Width of the wave packet increases with time ("Spreading of wave packet")

due to spread of $\psi(p)$ around p_0

→ Hamilton operator for a particle moving under the influence of an external force $F = -\frac{\partial}{\partial x} V(x)$: (1 dim.)

$$H = \frac{p^2}{2m} + V(x) \quad \Rightarrow \quad i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$$

$$\Rightarrow i\hbar \frac{d}{dt} \psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + V(x) \psi(x, t)$$

config space Schrödinger equation

↳ Important: The Hamilton operator H is / always must be a Hermitian operator!

→ Educational exercise:

Determine the form of the Schrödinger equation (with $V=0$) in momentum representation.

→ General approach for solving the Schrödinger equation:

$$\hookrightarrow \text{Formal solution: } |\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle$$

↪ Solve eigenvalue problem for H : $H|\psi\rangle = E|\psi\rangle$ (time-independent if $\frac{d}{dt}H = 0$!)

⇒ There is a Cols $\{|u\rangle\}$ of eigenvectors to the energy eigenvalues E_n to H :

$$H|u\rangle = E_n|u\rangle, \langle u|u\rangle = \delta_{uu}, \sum_n |u\rangle \langle u| = \mathbb{1}$$

↪ Spectral representations of Hamilton operator and time evolution operator:

$$H = \sum_n E_n |u\rangle \langle u|, e^{-iHt/\hbar} = \sum_n e^{-iE_n t/\hbar} |u\rangle \langle u|$$

↪ General form of solution:

$$|\psi(t)\rangle = \sum_n e^{-iE_n t/\hbar} |u\rangle \langle u| |\psi(0)\rangle$$

2.10. Probability Density and Probability Current

→ We already talked about the fact that probability in QM is a conserved quantity because the probability to get any result in a measurement is always 1 regardless of at what time one makes the measurement.

Important: For all conserved quantities one can define the concepts of "density", "total amount", "current" (other examples: energy, electric charge)

→ For a particle (free or in a potential V) we define the probability density as

$$S(x,t) := |\psi(x,t)|^2 \quad (1 \text{ dim})$$

↪ The time derivative of $S(x,t)$ is the rate of change in time of the probability density at location x:

$$\begin{aligned} \frac{d}{dt} S(x,t) &= \dot{\psi}^*(x,t) \psi(x,t) + \psi^*(x,t) \dot{\psi}(x,t) = -i\hbar (H\psi)^* \psi + i\hbar \psi^* (H\psi) \\ &= \frac{i\hbar}{2im} \left[\left(\frac{\partial^2}{\partial x^2} \psi \right)^* \psi - \psi^* \left(\frac{\partial^2}{\partial x^2} \psi \right) \right] \end{aligned}$$

$\downarrow H = \frac{p^2}{2m} + V$, V cancels

We can rewrite this as $\frac{\partial}{\partial t} S(x,t) + \frac{\partial}{\partial x} j_x(x,t) = 0$, called continuity equation for

$$j_x(x,t) := \frac{i\hbar}{2im} \left[\psi^*(x,t) \left(\frac{\partial}{\partial x} \psi(x,t) \right) - \left(\frac{\partial}{\partial x} \psi^*(x,t) \right) \psi(x,t) \right]$$

the probability current density.

→ The continuity equation expresses the conservation of probability in space and we:

$$w_I(t) = \int_a^b dx S(x,t) \quad \rightarrow \text{probability at time } t, \text{ that particle is in the interval } I = [a,b]$$

$$\frac{d}{dt} w_I(t) = \int_a^b dx \frac{\partial S(x,t)}{\partial t} \quad \rightarrow \text{rate of change of probability in time}$$

$$= - \int_a^b dx \frac{\partial j_x(x,t)}{\partial x}$$

$$= j_x(a,t) - j_x(b,t) \quad \rightarrow \text{current flowing into } I \text{ at a MINUS current flowing out of } I \text{ at } b$$

↪ The meaning of the continuity equation exactly expresses the conservation property in a local way: There is a change of the density $S(x,t)$ in time at x, if there is a difference in the currents that flow into x and flow out of x.

↪ Take limit $a \rightarrow -\infty$, $b \rightarrow +\infty$: Because the wave function vanishes for $|x| \rightarrow \infty$, we also have $\psi(x,t) \rightarrow 0$ for $|x| \rightarrow \infty$, so probability cannot escape at $|x| = \infty$.

$$\Rightarrow \frac{d}{dt} \int_{-\infty}^{+\infty} dx S(x,t) = 0$$

The equation exactly expresses the conservation property in a global way:

The amount of probability in all space (i.e. to find the particle anywhere in a measurement) does not change in time.

→ Generalization to 3 spatial dimensions:

$$S(\vec{x}, t) = |\psi(\vec{x}, t)|^2$$

prob. density

$$\vec{j}(\vec{x}, t) = \frac{\hbar}{2im} [\psi^*(\vec{x}, t) (\vec{\nabla} \psi(\vec{x}, t)) - (\vec{\nabla} \psi^*(\vec{x}, t)) \psi(\vec{x}, t)]$$

prob. current density

$$\frac{\partial}{\partial t} S(\vec{x}, t) + \vec{\nabla} \cdot \vec{j}(\vec{x}, t) = 0$$

continuity equation

$$\omega_v(t) = \int_{\mathbb{R}^3} d^3x S(\vec{x}, t), \quad V \subset \mathbb{R}^3$$

prob. to be found in region V

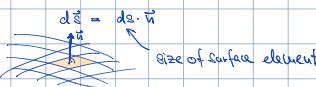
$$\frac{d}{dt} \omega_v(t) = \int_{\mathbb{R}^3} d^3x \frac{\partial S(\vec{x}, t)}{\partial t} = - \int_{\mathbb{R}^3} d^3x \vec{\nabla} \cdot \vec{j}(\vec{x}, t)$$

gaussian integration theorem

$$= - \int_V d\vec{s} \vec{j}(\vec{x}, t)$$

Surface
integral over V

infin. surface
element



$$\text{Limit } V \rightarrow \mathbb{R}^3: \text{ Because } \int_{\mathbb{R}^3} d^3x |\psi(\vec{x}, t)|^2 = \int_0^{2\pi} \int_0^\pi \int_0^\infty dr r^2 |\psi(\vec{x}, t)|^2 < \infty$$

we have $|\psi(\vec{x}, t)| \sim \frac{1}{|\vec{x}|^\alpha}$ for $|\vec{x}| \rightarrow \infty$ with $\alpha > \frac{3}{2}$

$\Rightarrow |\vec{j}| \sim \frac{1}{|\vec{x}|^\alpha}$ for $|\vec{x}| \rightarrow \infty$ with $\alpha > 4$

$$\Rightarrow \frac{d}{dt} \omega_v(t) = \lim_{V \rightarrow \mathbb{R}^3} \left[- \int_V d\vec{s} \vec{j}(\vec{x}, t) \right] \approx - \lim_{R \rightarrow \infty} \int d\Omega \cos \frac{R^2}{R^2} = 0$$

$\hookrightarrow \frac{d}{dt} \omega_{\mathbb{R}^3}(t) = 0$ total probability conservation

OR

conservation of the norm (in time)