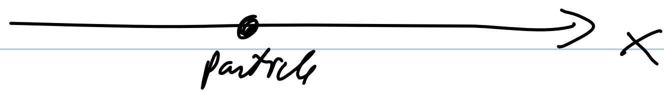
Chapter 6



$|\psi\rangle$

measurement of position:

basic event: find particle at position x

=> associated ket: $|x\rangle$ (label)
"position eigenstates"

- characterises the measurement outcome to detect particle at position x

position measurement gives mutual exclusive results

$\rightarrow \langle x | x' \rangle = 0$ for $x \neq x'$

	Discrete	Continuous
a) State	$\vert\Psi\rangle$	$\vert\Psi\rangle$
coordinate representation	$\vert\Psi\rangle \doteq \begin{pmatrix} \Psi_1 \\ \vdots \\ \Psi_n \end{pmatrix}$	$\vert\Psi\rangle \doteq \langle x\vert\Psi\rangle =: \Psi(x)$ wavefunction (complex valued!) (position representation)
completeness relations	$\mathbb{1} = \sum_{k=1}^{n} \vert\phi_k\rangle\langle\phi_k\vert$ orthonormal basis	$\mathbb{1} = \int_{-\infty}^{+\infty} dx\, \vert x\rangle\langle x\vert$ position states
dual vector	$\langle\Psi\vert \doteq \left(\Psi_1^*, \quad \ldots \quad \Psi_n^* \right)$	$\langle\Psi\vert \doteq \langle\Psi\vert x\rangle = \Psi(x)^*$
scalar product	$\langle\Phi\vert\Psi\rangle = \sum_{k=1}^{n} \Phi_k^* \Psi_k$	$\langle\Phi\vert\Psi\rangle = \int_{-\infty}^{+\infty} dx\, \Phi(x)^* \Psi(x)$
b) normalization	$1 \stackrel{!}{=} \langle\Psi\vert\Psi\rangle = \sum_{k=1}^{n} \vert\Psi_k\vert^2$	$1 \stackrel{!}{=} \langle\Psi\vert\Psi\rangle = \int_{-\infty}^{+\infty} dx\, \vert\Psi(x)\vert^2$
c) probability prediction	$\Pr(\text{"k"}) = \vert\langle\phi_k\vert\Psi\rangle\vert^2 = \vert\Psi_k\vert^2$ probability	$p(x)\, dx = \vert\langle x\vert\Psi\rangle\vert^2\, dx = \vert\Psi(x)\vert^2\, dx$ probability density

a)

The properties listed above can be easily derived using the completeness relations. Example:

Coordinate representation:

discrete

$$|\psi\rangle = \mathbb{1}|\psi\rangle = \sum_{k=1}^{n} |\phi_k\rangle \underbrace{\langle\phi_k|\psi\rangle}_{=:\,\psi_k \in \mathbb{C}}$$

$$= \sum_{k=1}^{n} \psi_k |\phi_k\rangle$$

$$|\psi\rangle \doteq \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_n \end{pmatrix}$$

continuous:

$$|\psi\rangle = \mathbb{1}|\psi\rangle = \int_{-\infty}^{+\infty} dx\ |x\rangle \underbrace{\langle x|\psi\rangle}_{\psi(x) \in \mathbb{C}}$$

$$= \int dx\ \psi(x)\ |x\rangle$$

$$|\psi\rangle \doteq \psi(x)$$

This is the wavefunction with respect to the position basis $|x\rangle$

It is an complex-valued function with a real parameter x.

discrete	continuous
$\vert\psi\rangle \doteq \psi_k$	$\vert\psi\rangle \doteq \psi(x)$

x plays in $\psi(x)$

the same role as the

index k in ψ_k

b) Normalization condition:
The normalization condition shows now that we encounter a new situation for continous systems.

Any vector $\begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix}$ (except the zero vector)

can be turned into a valid description of a quantum mechanical system by normalization, as the sum

$$\sum_{k=1}^{n} |\alpha_k|^2$$

always takes a definite finite value and so we can define

$$|\psi\rangle \doteq \frac{1}{\sqrt{\sum_{k=1}^{n} |\alpha_k|^2}} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix}$$

In the continuous case, we cannot turn any function f(x) into a position wave-function by normalization.
For example the assignment

$$|\psi\rangle \doteq \frac{1}{\sqrt{\int_{-\infty}^{+\infty} dx' |f(x')|^2}} f(x)$$

fails if the integral $\int_{-\infty}^{+\infty} dx \; |f(x')|^2$ fails to converge.

(Try with f(x) = x^2)

c) Probability prediction
discrete:
Here we have the basic postulate that

$$Pr(\text{“}k\text{''}) = |\langle \phi_k | \psi \rangle|^2$$

continuous:
The above concept does not work that easy if we go to continuous distributions, as the probability to find mathematically exact one particular value of x will be zero.

The proper question is to ask what the probability is to find the value of x in a given interval, for example

$$x \in [x, x+\Delta] \quad \text{for some } \Delta > 0$$

and our postulate now takes the form

$$\int_x^{x+\Delta} dx \; |\langle x|\psi\rangle|^2 = \int_x^{x+\Delta} dx \; |\psi(x)|^2 dx$$

so instead of probabilities as underlying quantity, in continuous systems we use probability densities p(x)
where quantum mechanics assigns $p(x) = |\psi(x)|^2$

(For more about probability densities, see McIntyre, Appendix A.2)

6.2 Position operator

6.2.1 Definition

probability to find particle in interval [x,x+dx] :

$$p(x)\,dx = |\psi(x)|^2 dx$$

mean value of position:

$$\langle x\rangle := \int dx \; x\, p(x) = \int dx \; x\, |\psi(x)|^2$$

Similarly:

$$\langle x^2\rangle := \int dx \; x^2 \, |\psi(x)|^2 dx$$

We can reformulate this as:

$$\langle x\rangle = \int dx \; x\, |\langle x|\psi\rangle|^2 dx$$

$$= \langle \psi | \underbrace{\left(\int dx \; x \, |x\rangle\langle x| \right)}_{=: \hat{X}} |\psi\rangle$$

$$= \langle \psi | \hat{X} | \psi \rangle \equiv \langle \hat{X} \rangle$$

NOTATION: since we have many x's flying around:
the 'hat' $\hat{}$ on a symbol emphasizes the operator nature. I will use it wherever it might be ambiguous whether I refer to the operator or to a variable (scalar)

example $$\hat{X} = \int_{-\infty}^{+\infty} dx \; x \, |x\rangle\langle x|$$

operator

variable (scalar)

ket
bra
which use x as index!

$$\boxed{\text{Position operator} \quad \hat{X} = \int dx \; x \, |x\rangle\langle x|}$$

Similarly we find the operator

$$\widehat{(X^2)} = \int dx \; x^2 \, |x\rangle\langle x|$$

6.2.2 Coordinate representation

We need to get the proper coordinate representations of our operators so that we can translate all knowledge straightforwardly form the finite dimensional case to the new infinite dimensional case!

In finite dimension we have for an operator on a d-dimensional complex vector space:

$$\hat{A} = \mathbb{1} \hat{A} \mathbb{1}$$

$$= \sum_{k=1}^{d} |\varphi_k\rangle\langle\varphi_k| \hat{A} \sum_{\ell=1}^{d} |\varphi_\ell\rangle\langle\varphi_\ell|$$

$$= \sum_{k=1}^{d} \sum_{\ell=1}^{d} |\varphi_k\rangle \underbrace{\langle\varphi_k| \hat{A} |\varphi_\ell\rangle}_{=: \alpha_{k\ell}} \langle\varphi_\ell|$$

$$= \sum_{\substack{k=1 \\ l=1}}^{d} \alpha_{kl} \, |\varphi_k\rangle\langle\varphi_l|$$

so that α_{kl} is the coordinate representation of the operator $\hat{A}$, and we think about this number as the matrix representing the operator.

Similarly, in infinite dimensions we have for an operator $\hat{B}$ acting on that space:

$$\hat{B} = \mathbb{1}\,\hat{B}\,\mathbb{1}$$

$$= \int_{-\infty}^{+\infty} dx \, |x\rangle\langle x| \, \hat{B} \int_{-\infty}^{+\infty} dx' \, |x'\rangle\langle x'|$$

$$= \int_{-\infty}^{+\infty}\!\!\int dx \, dx' \; |x\rangle \; \underbrace{\langle x|\hat{B}|x'\rangle}_{=: f(x,x')} \langle x'|$$

$$= \int_{-\infty}^{+\infty}\!\!\int dx \, dx' \; |x\rangle \; f(x,x') \, \langle x'|$$

where the function f(x,x') is now the coordinate representation of the operator B with respect to the position basis $|x\rangle$.

Usage: Evaluation of expectation values

If we want to evaluate the expectation value of an operator, we can do so as follows:

$$\langle\psi| \underset{\mathbb{1}}{\wedge} \hat{B} \underset{\mathbb{1}}{\wedge} |\psi\rangle = \langle\psi| \int_{-\infty}^{+\infty} dx \, |x\rangle\langle x| \, \hat{B} \int_{-\infty}^{+\infty} dx' \, |x'\rangle\langle x'|\psi\rangle$$

$$= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dx \, dx' \; \langle\psi|x\rangle\langle x|\hat{B}|x'\rangle\langle x'|\psi\rangle$$

$$= \iint_{-\infty}^{+\infty} dx\, dx' \; \psi^*(x)\, f(x,x')\, \psi(x)$$

which is the anlogue of the finite dimensional case:

$$\langle \psi | A | \psi \rangle = \sum_{k,l=1}^{d} \psi_k^* A_{kl} \psi_l$$

$$A_{kl} = {}_d\langle \varphi_k | A | \varphi_l \rangle$$

$$|\psi\rangle = \sum_{l=1}^{d} \psi_l \, |\varphi_l\rangle$$

6.2.3 Coordinate representation of Position operator

The form of the position operator

$$\hat{X} = \int_{-\infty}^{+\infty} dx \; x \; |x\rangle\langle x|$$

looks close to what we want, namely an expression

$$\hat{X} = \iint_{-\infty}^{+\infty} dx\, dx' \; g(x,x') \; |x\rangle\langle x'|$$

but not quite ...   The first form looks actually like the representation of an operator in the eigenbasis of the operator!

in finite dimensions we have for the eigenbasis

$$A = \sum_{i=1}^{d} \lambda_i \, |\lambda_i\rangle\langle\lambda_i|$$

In order to calcuate the coordinate representation g(x,x'), which should be a complex valued function of the two real variables x and x', let us calculate

$$\langle x|A|x'\rangle = \langle x|\left[\int_{-\infty}^{+\infty} dx''\, x''\, |x''\rangle\langle x''|\right]|x'\rangle$$

$$= \int_{-\infty}^{+\infty} dx''\, x''\, \langle x|x''\rangle \langle x''|x'\rangle$$

To evaluate this, we need to know what the overlap between two position states are:

$$\langle x|x''\rangle = \begin{cases} 0 & x \neq x'' \\ ? & x = x'' \end{cases}$$

It turns out, that we cannot choose

$$\langle x|x''\rangle = 1 \quad \text{for } x = x''$$

The integration would always give zero, as the overlap functions are different from zero only in single points!

The answer is given via the Dirac delta function, and we need that to stay consistent.

This special role is actually a consequence that the states are not proper physical states. The do not have normalizable wave functions....

So we will never write that we prepare a system in the state

$$\cancel{|\psi\rangle = |x\rangle}$$

Still, they form a very convenient tool as a convenient basis to work with! For this tool, we don't worry that we can't normalize them.