# Quantum Mechanics: Change of basis

## Transforming bases

By now we have learnt that eigenstates of a Hermitian operator form a complete set, and can be used as basis states to represent any arbitrary state. Consider two Hermitian operators $\hat{A}$ and $\hat{B}$, and their corresponding eigenstates and eigenvalues

$$\hat{A}|a_n\rangle = \alpha_n|a_n\rangle, \qquad \hat{B}|b_n\rangle = \beta_n|b_n\rangle.$$

A state $|\psi\rangle$ can be expanded in terms of both the set of states, $\{|a_n\rangle\}$ and $\{|b_n\rangle\}$

$$|\psi\rangle = \sum_n c_n|a_n\rangle, \qquad |\psi\rangle = \sum_n d_n|b_n\rangle.$$

Now, the question we ask is, how can one go from the set $\{|a_n\rangle\}$ to $\{|b_n\rangle\}$? The answer is that **there exists a unitary operator that takes each state of one basis to a state of another basis.** The mathematical content of the statement is

$$|b_k\rangle = \hat{U}|a_k\rangle,$$

for all $k$. We can prove this assertion by a specific construction:

$$\hat{U} = \sum_n |b_n\rangle\langle a_n|.$$

But first we should prove that this $\hat{U}$ is really a unitary operator. For that we find the adjoint of $\hat{U}$

$$\begin{aligned}\langle\psi|\hat{U}^\dagger|\phi\rangle = \langle\phi|\hat{U}|\psi\rangle^* &= \sum_n \left(\langle\phi|b_n\rangle\langle a_n|\psi\rangle\right)^* \\ &= \sum_n \langle\psi|a_n\rangle\langle b_n|\phi\rangle = \langle\psi|\sum_n |a_n\rangle\langle b_n|\,|\phi\rangle. \end{aligned} \tag{1}$$

Comparing the LHS and RHS, we infer that

$$\hat{U}^\dagger = \sum_n |a_n\rangle\langle b_n|.$$

Now to test if it is unitary

$$\begin{aligned}\hat{U}^\dagger\hat{U} &= \sum_n |a_n\rangle\langle b_n| \sum_m |b_m\rangle\langle a_m| = \sum_{n,m} |a_n\rangle\delta_{nm}\langle a_m| \\ &= \sum_n |a_n\rangle\langle a_n| = \hat{1}, \end{aligned} \tag{2}$$

which means $\hat{U}$ is unitary. Now to check if it does the job of changing the basis, we let it act on a basis state

$$\hat{U}|a_k\rangle = \sum_n |b_n\rangle\langle a_n|a_k\rangle = \sum_n |b_n\rangle\delta_{nk} = |b_k\rangle.$$

We see that $\hat{U}$ does transform $|a_k\rangle$ to $|b_k\rangle$.

## Trace is basis independent

We can apply what we have just learnt in proving that trace is independent of the basis used. Trace of an operator $\hat{Q}$, taken in a basis $\{|b_j\rangle\}$, is given by

$$
\begin{aligned}
\sum_j \langle b_j|\hat{Q}|b_j\rangle &= \sum_j \langle a_j|\hat{U}^\dagger\hat{Q}\hat{U}|a_j\rangle \\
&= \sum_j \langle a_j|\hat{U}^\dagger \sum_k |a_k\rangle\langle a_k|\hat{Q}\hat{U}|a_j\rangle \\
&= \sum_{jk} \langle a_k|\hat{Q}\hat{U}|a_j\rangle\langle a_j|\hat{U}^\dagger|a_k\rangle \\
&= \sum_k \langle a_k|\hat{Q}\hat{U}\hat{U}^\dagger|a_k\rangle \\
&= \sum_k \langle a_k|\hat{Q}|a_k\rangle. \qquad (3)
\end{aligned}
$$

## Continuous basis: Position & momentum eigenstates

In quantum mechanics one often deals with set of states which are not discrete, but continuous. For such situations it is common to use eigenstates of position and momentum operators, which we denote by $\hat{X}$ and $\hat{P}$. Eigenstates of the two operators can be written as

$$\hat{X}|x'\rangle = x'|x'\rangle \qquad \hat{P}|p'\rangle = p'|p'\rangle,$$

where $x', p'$ are the respective eigenvalues. Since $\{|x\rangle\}$ and $\{|p\rangle\}$ are not discrete, but continuous set of states, the completeness relation will not involve a sum, but integral:

$$\int_{-\infty}^{\infty} |x'\rangle\langle x'|dx' = \hat{1} \qquad \int_{-\infty}^{\infty} |p'\rangle\langle p'|dp' = \hat{1}.$$

The orthonormality condition too will no longer involve a Kronecker delta, but the Dirac delta function:

$$\langle x'|x\rangle = \delta(x - x') \qquad \langle p'|p\rangle = \delta(p - p').$$

A state $|\psi\rangle$ can now be represented in the position basis by simply letting the above unit operator act on it:

$$|\psi\rangle = \int_{-\infty}^{\infty} |x'\rangle\langle x'|dx'|\psi\rangle = \int_{-\infty}^{\infty} |x'\rangle\langle x'|\psi\rangle dx'.$$

Now $\langle x|\psi\rangle$ is what we have been representing as $\psi(x)$, the wave-function. We can now see the precise relation between ket states and the wave-functions, which we introduced earlier in a loose manner:

$$\boxed{\psi(x) = \langle x|\psi\rangle \qquad |\psi\rangle = \int_{-\infty}^{\infty} \psi(x)|x\rangle dx.}$$

We can also write the norm of $|\psi\rangle$ using the position basis, by introducing a complete set in between

$$\langle\psi|\psi\rangle = \langle\psi| \int_{-\infty}^{\infty} |x\rangle\langle x|dx|\psi\rangle = \int_{-\infty}^{\infty} \langle\psi|x\rangle\langle x|\psi\rangle dx =$$

which yields our original normalization relation

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1.$$

Similary we can write for momentum eigenstates:

$$\tilde{\psi}(p) = \langle p|\psi\rangle \qquad |\psi\rangle = \int_{-\infty}^{\infty} \tilde{\psi}(p)|p\rangle dp,$$

where the “tilde” in $\tilde{\psi}(p)$ has been introduced to emphasize that it has a functional form different from $\psi(x)$. The function $\tilde{\psi}(p)$ is referred to as the *wave-function in momentum basis*.

## Transforming between position & momentum bases

Given the position space wave-function $\psi(x)$ for a state $|\psi\rangle$, let us find out how we can find the *momentum space* wave-function $\tilde{\psi}(p)$. We know that the momentum space wave-function is given by $\tilde{\psi}(p) = \langle p|\psi\rangle$. We will start by inserting a complete set of position eigenstates on the RHS:

$$\begin{aligned}\tilde{\psi}(p) &= \langle p|\int_{-\infty}^{\infty} |x\rangle\langle x|dx|\psi\rangle \\ &= \int_{-\infty}^{\infty} \langle p|x\rangle\langle x|\psi\rangle dx = \int_{-\infty}^{\infty} \phi_p^*(x)\psi(x)dx, \end{aligned} \tag{4}$$

where $\phi_p(x)$ are eigenfunctions of the momentum operator, in the position basis, i.e., $\hat{P}\phi_p(x) = p\phi_p(x)$. These can be easily obtained by solving this equation

$$-i\hbar\frac{d\phi_p(x)}{dx} = p\phi_p(x).$$

The result is $\phi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}$. Substituting this in (4) we get

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\psi(x)dx.$$

We now understand the origin of this familiar relation.

Transformation in the other direction can be similarly obtained.

$$
\begin{aligned}
\psi(x) = \langle x|\psi\rangle &= \langle x| \int_{-\infty}^{\infty} |p\rangle\langle p| dp |\psi\rangle \\
&= \int_{-\infty}^{\infty} \langle x|p\rangle\langle p|\psi\rangle dp = \int_{-\infty}^{\infty} \phi_p(x)\tilde{\psi}(p) dp \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar}\tilde{\psi}(p) dp
\end{aligned}
\tag{5}
$$