Translations

The previous discrete spectrum state vector formalism can be generalized also to continuos cases, in practice, by replacing

- summations with integrations
- Kronecker's δ-function with Dirac's δ-function.

A typical continuous case is the measurement of position:

- the operator x corresponding to the measurement of the x-coordinate of the position is Hermitean,
- the eigenvalues $\{x'\}$ of x are real,
- the eigenvectors $\{|x'\rangle\}$ form a complete basis.

So, we have

$$\begin{aligned} x|x'\rangle &= x'|x'\rangle \\ 1 &= \int_{-\infty}^{\infty} dx'\, |x'\rangle\langle x'| \\ |\alpha\rangle &= \int_{-\infty}^{\infty} dx'\, |x'\rangle\langle x'|\alpha\rangle, \end{aligned}$$

where $|\alpha\rangle$ is an arbitrary state vector. The quantity $\langle x'|\alpha\rangle$ is called a *wave function* and is usually written down using the function notation

$$\langle x'|\alpha\rangle = \psi_\alpha(x').$$

Obviously, looking at the expansion

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

the quantity $|\psi_\alpha(x')|^2 dx'$ can be interpreted according to the postulate 3 as the probability for the state being localized in the neighborhood $(x', x' + dx')$ of the point x'.

The position can be generalized to three dimension. We denote by $|\boldsymbol{x}'\rangle$ the *simultaneous* eigenvector of the operators x, y and z, i.e.

$$\begin{aligned} |\boldsymbol{x}'\rangle &\equiv |x', y', z'\rangle \\ x|\boldsymbol{x}'\rangle &= x'|\boldsymbol{x}'\rangle, \quad y|\boldsymbol{x}'\rangle = y'|\boldsymbol{x}'\rangle, \quad z|\boldsymbol{x}'\rangle = z'|\boldsymbol{x}'\rangle. \end{aligned}$$

The exsistence of the common eigenvector requires commutativity of the corresponding operators:

$$[x_i, x_j] = 0.$$

Let us suppose that the state of the system is localized at the point $\boldsymbol{x}'$. We consider an operation which transforms this state to another state, this time localized at the point $\boldsymbol{x}' + d\boldsymbol{x}'$, all other observables keeping their values. This operation is called an *infinitesimal translation*. The corresponding operator is denoted by $\mathcal{T}(d\boldsymbol{x}')$:

$$\mathcal{T}(d\boldsymbol{x}')|\boldsymbol{x}'\rangle = |\boldsymbol{x}' + d\boldsymbol{x}'\rangle.$$

The state vector on the right hand side is again an eigenstate of the position operator. Quite obviously, the vector $|\boldsymbol{x}'\rangle$ is *not* an eigenstate of the operator $\mathcal{T}(d\boldsymbol{x}')$.

The effect of an infinitesimal translation on an arbitrary state can be seen by expanding it using position eigenstates:

$$\begin{aligned}
|\alpha\rangle \longrightarrow \mathcal{T}(d\boldsymbol{x}'')|\alpha\rangle &= \mathcal{T}(d\boldsymbol{x}'')\int d^3x'\,|\boldsymbol{x}'\rangle\langle\boldsymbol{x}'|\alpha\rangle \\
&= \int d^3x'\,|\boldsymbol{x}' + d\boldsymbol{x}''\rangle\langle\boldsymbol{x}'|\alpha\rangle \\
&= \int d^3x'\,|\boldsymbol{x}'\rangle\langle\boldsymbol{x}' - d\boldsymbol{x}''|\alpha\rangle,
\end{aligned}$$

because $\boldsymbol{x}'$ is an ordinary integration variable.

To construct $\mathcal{T}(d\boldsymbol{x}')$ explicitely we need extra constraints:

1. it is natural to require that it preserves the normalization (i.e. the conservation of probability) of the state vectors:

   $$\langle\alpha|\alpha\rangle = \langle\alpha|\mathcal{T}^\dagger(d\boldsymbol{x}')\mathcal{T}(d\boldsymbol{x}')|\alpha\rangle.$$

   This is satisfied if $\mathcal{T}(d\boldsymbol{x}')$ is unitary, i.e.

   $$\mathcal{T}^\dagger(d\boldsymbol{x}')\mathcal{T}(d\boldsymbol{x}') = 1.$$

2. we require that two consecutive translations are equivalent to a single combined transformation:

   $$\mathcal{T}(d\boldsymbol{x}')\mathcal{T}(d\boldsymbol{x}'') = \mathcal{T}(d\boldsymbol{x}' + d\boldsymbol{x}'').$$

3. the translation to the opposite direction is equivalent to the inverse of the original translation:

   $$\mathcal{T}(-d\boldsymbol{x}') = \mathcal{T}^{-1}(d\boldsymbol{x}').$$

4. we end up with the identity operator when $d\boldsymbol{x}' \to 0$:

   $$\lim_{d\boldsymbol{x}'\to 0} \mathcal{T}(d\boldsymbol{x}') = 1.$$

It is easy to see that the operator

$$\mathcal{T}(d\boldsymbol{x}') = 1 - i\boldsymbol{K}\cdot d\boldsymbol{x}',$$

where the components K_x, K_y and K_z of the vector $\boldsymbol{K}$ are *Hermitean operators*, satisfies all four conditions. Using the definition

$$\mathcal{T}(d\boldsymbol{x}')|\boldsymbol{x}'\rangle = |\boldsymbol{x}' + d\boldsymbol{x}'\rangle$$

we can show that

$$[\boldsymbol{x}, \mathcal{T}(d\boldsymbol{x}')] = d\boldsymbol{x}'.$$

Substituting the explicit representation

$$\mathcal{T}(d\boldsymbol{x}') = 1 - i\boldsymbol{K}\cdot d\boldsymbol{x}'$$

it is now easy to prove the commutation relation

$$[x_i, K_j] = i\delta_{ij}.$$

The equations

$$\begin{aligned}\mathcal{T}(d\boldsymbol{x}') &= 1 - i\boldsymbol{K}\cdot d\boldsymbol{x}' \\ \mathcal{T}(d\boldsymbol{x}')|\boldsymbol{x}'\rangle &= |\boldsymbol{x}' + d\boldsymbol{x}'\rangle\end{aligned}$$

can be considered as the definition of $\boldsymbol{K}$.
One would expect the operator $\boldsymbol{K}$ to have something to do with the momentum. It is, however, not quite the momentum, because its dimension is 1/length. Writing

$$\boldsymbol{p} = \hbar\boldsymbol{K}$$

we get an operator $\boldsymbol{p}$, with dimension of momentum.

- We borrow the name "momentum" from classical physics and
- define momentum as the the generator of infinitesimal translation

The commutation relation

$$[x_i, K_j] = i\delta_{ij}$$

can now be written in a familiar form like

$$[x_i, p_j] = i\hbar\delta_{ij}.$$

Accordingly, for example x_x and p_x are incompatible observables while x_x and p_y are compatible and thus it is impossible to find simultaneous eigenkets of x and p_x.
$\Rightarrow$ <u>uncertainty relation</u>

Finite translations
Consider translation of the distance $\Delta x'$ along the x-axis:

$$\mathcal{T}(\Delta x'\hat{\boldsymbol{x}})|\boldsymbol{x}'\rangle = |\boldsymbol{x}' + \Delta x'\hat{\boldsymbol{x}}\rangle.$$

We construct this translation combining infinitesimal translations of distance $\Delta x'/N$ letting $N \to \infty$:

$$\begin{aligned} \mathcal{T}(\Delta x' \hat{\boldsymbol{x}}) &= \lim_{N\to\infty} \left(1 - \frac{ip_x \Delta x'}{N\hbar}\right)^N \\ &= \exp\left(-\frac{ip_x \Delta x'}{\hbar}\right). \end{aligned}$$

The exponential is *an operator* and must be expanded when applied on a ket. It is relatively easy to show that the translation operators satisfy

$$[\mathcal{T}(\Delta y' \hat{\boldsymbol{y}}), \mathcal{T}(\Delta x' \hat{\boldsymbol{x}})] = 0,$$

so it follows that

$$[p_y, p_x] = 0.$$

Generally

$$[p_i, p_j] = 0.$$

This commutation relation tells that it is possible to construct a state vector which is a simultaneous eigenvector of all components of the momentum operator, i.e. there exists a vector

$$|\boldsymbol{p}'\rangle \equiv |p'_x, p'_y, p'_z\rangle,$$

so that

$$p_x|\boldsymbol{p}'\rangle = p'_x|\boldsymbol{p}'\rangle, \quad p_y|\boldsymbol{p}'\rangle = p'_y|\boldsymbol{p}'\rangle, \quad p_z|\boldsymbol{p}'\rangle = p'_z|\boldsymbol{p}'\rangle.$$

The effect of the translation $\mathcal{T}(d\boldsymbol{x}')$ on an eigenstate of the momentum operator is

$$\mathcal{T}(d\boldsymbol{x}')|\boldsymbol{p}'\rangle = \left(1 - \frac{i\boldsymbol{p}\cdot d\boldsymbol{x}'}{\hbar}\right)|\boldsymbol{p}'\rangle = \left(1 - \frac{i\boldsymbol{p}'\cdot d\boldsymbol{x}'}{\hbar}\right)|\boldsymbol{p}'\rangle.$$

The state $|\boldsymbol{p}'\rangle$ is thus an eigenstate of $\mathcal{T}(d\boldsymbol{x}')$: a result, which we could have predicted because

$$[\boldsymbol{p}, \mathcal{T}(d\boldsymbol{x}')] = 0.$$

Note The eigenvalues of $\mathcal{T}(d\boldsymbol{x}')$ are complex because it is not Hermitean.
So, we have derived the *canonical commutation relations* or *fundamental commutation relations:*

$$[x_i, x_j] = 0, \quad [p_i, p_j] = 0, \quad [x_i, p_j] = i\hbar\delta_{ij}.$$

Home work: Refresh your memory about what you have learned about canonical commutation relations and previously derived identities.

Wave functions, position space

Recall, that the projection $\langle x'|\alpha\rangle$ of the state $|\alpha\rangle$ along the state vector $|x'\rangle$ was called the *wave function* and was denoted like $\psi_\alpha(x')$. Since the vectors $|x'\rangle$ form a complete basis the scalar product between the states $|\alpha\rangle$ and $|\beta\rangle$ can be written with the help of the wave functions as

$$\langle\beta|\alpha\rangle = \int dx'\, \langle\beta|x'\rangle\langle x'|\alpha\rangle = \int dx'\, \psi_\beta^*(x')\psi_\alpha(x'),$$

i.e.

$\langle\beta|\alpha\rangle$ tells how much the wave functions overlap.

If $|a'\rangle$ is an eigenstate of A we define the corresponding *eigenfunction* $u_{a'}(x')$ like

$$u_{a'}(x') = \langle x'|a'\rangle.$$

An arbitrary wave function $\psi_\alpha(x')$ can be expanded using eigenfunctions as

$$\psi_\alpha(x') = \sum_{a'} c_{a'} u_{a'}(x').$$

since $|\alpha\rangle=\sum_{a'}|a'\rangle\langle a'|\alpha\rangle = \sum_{a'} c_{a'}|a'\rangle$
$\langle x'|\alpha\rangle = \psi_\alpha(x') = \sum_{a'} c_{a'}\langle x'|a'\rangle = \sum_{a'} c_{a'}u_{a'}(x')$

The matrix element $\langle\beta|A|\alpha\rangle$ of an operator A can also be expressed with the help of eigenfunctions like

$$\begin{aligned}\langle\beta|A|\alpha\rangle &= \int dx' \int dx''\, \langle\beta|x'\rangle\langle x'|A|x''\rangle\langle x''|\alpha\rangle \\ &= \int dx' \int dx''\, \psi_\beta^*(x')\langle x'|A|x''\rangle\psi_\alpha(x'').\end{aligned}$$

To apply this formula we have to evaluate the matrix elements $\langle x'|A|x''\rangle$, which in general are functions of the two variables x' and x''. When A depends only on the position operator x,

$$A = f(x),$$

the calculations are much simpler since the matrix element reduces to a single integral:

$$\langle\beta|f(x)|\alpha\rangle = \int dx'\, \psi_\beta^*(x')f(x')\psi_\alpha(x').$$

Note $f(x)$ on the left hand side is an operator while $f(x')$ on the right hand side is an ordinary number.

Example $f(x) = x^2$

$$\begin{aligned}
\langle x'|x^2|x''\rangle &= \langle x'|xx''|x''\rangle = \langle x'|(x'')^2|x''\rangle \\
&= (x'')^2\langle x'|x''\rangle \\
\langle \beta|x^2|\alpha\rangle &= \int x''^2 dx' \int dx'' \psi_\beta^*(x')\langle x'|x''\rangle\psi_\alpha(x'') \\
&= \int x'^2 \psi_\beta^*(x')\psi_\alpha(x')dx'
\end{aligned}$$

Momentum operator $\boldsymbol{p}$ in position basis $\{|\boldsymbol{x}'\rangle\}$
For simplicity we consider the one dimensional case. According to the equation

$$\begin{aligned}
\mathcal{T}(d\boldsymbol{x}'')|\alpha\rangle &= \mathcal{T}(d\boldsymbol{x}'') \int d^3x'\, |\boldsymbol{x}'\rangle\langle \boldsymbol{x}'|\alpha\rangle \\
&= \int d^3x'\, |\boldsymbol{x}' + d\boldsymbol{x}''\rangle\langle \boldsymbol{x}'|\alpha\rangle \\
&= \int d^3x'\, |\boldsymbol{x}'\rangle\langle \boldsymbol{x}' - d\boldsymbol{x}''|\alpha\rangle
\end{aligned}$$

we can write

$$\begin{aligned}
&\left(1 - \frac{ip\,dx''}{\hbar}\right)|\alpha\rangle \\
&= \int dx'\, \mathcal{T}(dx'')|x'\rangle\langle x'|\alpha\rangle \\
&= \int dx'\, |x'\rangle\langle x' - dx''|\alpha\rangle \\
&= \int dx'\, |x'\rangle \left(\langle x'|\alpha\rangle - dx''\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right).
\end{aligned}$$

In the last step we have expanded $\langle x' - dx''|\alpha\rangle$ as Taylor series. Comparing both sides of the equation we see that

$$p|\alpha\rangle = \int dx'\, |x'\rangle \left(-i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right),$$

or, taking scalar product with a position eigenstate on both sides,

$$\langle x'|p|\alpha\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle.$$

In particular, if we choose $|\alpha\rangle = |x''\rangle$ we get

$$\langle x'|p|x''\rangle = -i\hbar\frac{\partial}{\partial x'}\delta(x' - x'').$$

Taking scalar product with an arbitrary state vector $|\beta\rangle$ on both sides of

$$p|\alpha\rangle = \int dx'\,|x'\rangle\left(-i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right)$$

we get the important identity:

$$\langle\beta|p|\alpha\rangle = \int dx'\psi^*_\beta(x')\left(-i\hbar\frac{\partial}{\partial x'}\right)\psi_\alpha(x').$$

Wave functions, momentum space
Just like the position eigenvalues also the momentum eigenvalues p' comprise a continuum. Thus, we can work in the p-basis equally well by specifying the base eigenkets in the p-basis:

$$\begin{aligned} p|p'\rangle &= p'|p'\rangle \\ \langle p'|p''\rangle &= \delta(p'-p'') \end{aligned}$$

Analogically we can define the *momentum space wave function* as

$$\langle p'|\alpha\rangle = \phi_\alpha(p').$$

We can move between the momentum and configuration space representations with help of the relations

$$\begin{aligned} \psi_\alpha(x') &= \langle x'|\alpha\rangle &= \int dp'\,\langle x'|p'\rangle\langle p'|\alpha\rangle \\ \phi_\alpha(p') &= \langle p'|\alpha\rangle &= \int dx'\,\langle p'|x'\rangle\langle x'|\alpha\rangle. \end{aligned}$$

The transformation function $\langle x'|p'\rangle$ can be evaluated by substituting a momentum eigenvector $|p'\rangle$ for $|\alpha\rangle$ into

$$\langle x'|p|\alpha\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle.$$

Then

$$\langle x'|p|p'\rangle = p'\langle x'|p'\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|p'\rangle.$$

The solution of this differential equation is

$$\langle x'|p'\rangle = C\exp\left(\frac{ip'x'}{\hbar}\right),$$

where the normalization factor C can be determined from the identity

$$\begin{aligned} \langle x'|x''\rangle &= \int dp'\,\langle x'|p'\rangle\langle p'|x''\rangle \\ \delta(x'-x'') &= 2\pi\hbar|C|^2\delta(x'-x'') \\ \Rightarrow C &= \frac{1}{\sqrt{2\pi\hbar}} \end{aligned}$$

since

$$\begin{aligned}
\langle x'|p'\rangle\langle p'|x''\rangle &= C\exp\left(\frac{ip'x'}{\hbar}\right)C^*\exp\left(\frac{-ip'x''}{\hbar}\right)\\
&= |C|^2\exp\left(\frac{ip'(x'-x'')}{\hbar}\right) \quad \text{and}\\
\delta(f) &= \int_{-\infty}^{\infty} e^{2\pi i f y}dy
\end{aligned}$$

Thus the transformation function is

$$\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left(\frac{ip'x'}{\hbar}\right),$$

and the relations

$$\begin{aligned}
\psi_\alpha(x') &= \langle x'|\alpha\rangle &= \int dp'\,\langle x'|p'\rangle\langle p'|\alpha\rangle\\
\phi_\alpha(p') &= \langle p'|\alpha\rangle &= \int dx'\,\langle p'|x'\rangle\langle x'|\alpha\rangle.
\end{aligned}$$

can be written as familiar Fourier transforms

$$\begin{aligned}
\psi_\alpha(x') &= \left[\frac{1}{\sqrt{2\pi\hbar}}\right]\int dp'\,\exp\left(\frac{ip'x'}{\hbar}\right)\phi_\alpha(p')\\
\phi_\alpha(p') &= \left[\frac{1}{\sqrt{2\pi\hbar}}\right]\int dx'\,\exp\left(-\frac{ip'x'}{\hbar}\right)\psi_\alpha(x').
\end{aligned}$$

Generalization to 3-dimensional case is straight forward:

$$\begin{aligned}
\delta &\rightarrow \delta^3\\
\partial/\partial_x &\rightarrow \nabla\\
\sqrt{2\pi\hbar} &\rightarrow \sqrt{2\pi\hbar}^3\\
p'x' &\rightarrow \mathbf{p}'\cdot\mathbf{x}'
\end{aligned}$$

Uncertainty relation
Corresponding to an observable $\mathcal{A}$, let us define an operator

$$\Delta A = A - \langle A\rangle$$

The dispersion
(aka variance aka mean square deviation) reads

$$\begin{aligned}
\langle(\Delta A)^2\rangle &= \langle(A^2 - 2A\langle A\rangle + \langle A\rangle^2)\rangle\\
&= \langle A^2\rangle - \langle A\rangle^2
\end{aligned}$$

Generalized uncertanty relation:

Let $\mathcal{A}$ and $\mathcal{B}$ be observables corresponding to operators A and B. Then for any state following inequality must hold:

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A,B]\rangle|^2$$

Proof of this is straight forward and can be found for example from Sakurai's book page 35.
At blackboard, we will show that for a gaussian wave packet

$$\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle = \frac{\hbar^2}{4}$$

Notice that gaussian wave packet is often referred as *minimum uncertainty wave packet*
Alternatively we could have worked in the momentum space by obtaining the momentum space wave functions from

$$\langle p'|\alpha\rangle \quad = \quad \int dx' \, \langle p'|x'\rangle\langle x'|\alpha\rangle$$

Notice, the uncertainty relation could have been derived directly from the properties of Fourier transformations, since it can be shown that for (properly normalized) Fourier transformations

$$X(w) = \int x(t)e^{-iwt}dt,$$

the following holds

$$\Delta t \Delta w \geq \frac{1}{2}$$