Continuum bases

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The bra-ket notation applies equally well to both discrete and continuum bases, the only major changes being that sums are replaced by integrals and Kronecker deltas become Dirac deltas. Here is a full set of correspondences:

State	$\|\chi\rangle$	$\|\psi\rangle$
Basis	$\|a'\rangle$	$\|\xi\rangle$
Eigenstate	$\hat{\mathcal{O}}\|a'\rangle = a'\|a'\rangle$	$\hat{\mathcal{O}}\|\xi'\rangle = \xi'\|\xi'\rangle$
Identity	$\hat{1} = \sum_{a'}\|a'\rangle\langle a'\|$	$\hat{1} = \int d\xi\,\|\xi\rangle\langle\xi\|$
Completeness	$\sum_{a'}\langle a'\|\,a''\rangle = \delta_{a'a''}$	$\int d\xi'\,\langle\xi'\|\,\xi''\rangle = \delta(\xi'-\xi'')$
State in basis	$\|\chi\rangle = \sum_{a'}\|a'\rangle\langle a'\|\,\chi\rangle$	$\|\psi\rangle = \int d\xi'\,\|\xi'\rangle\langle\xi'\|\,\psi\rangle$
Operator	$\hat{\mathcal{O}} = \sum_{a'} a'\|a'\rangle\langle a'\|$	$\hat{\mathcal{O}} = \int d\xi'\xi'\,\|\xi'\rangle\langle\xi'\|$
Matrix element	$\langle a'\|\,\hat{\mathcal{O}}\,\|a''\rangle$	$\langle\xi'\|\,\hat{\mathcal{O}}\,\|\xi''\rangle$

In a continuous basis, the expansion coefficients of states are *functions*,

$$\langle\xi'|\,\psi\rangle = \psi(\xi')$$

and the bra-ket notation allows us to talk about the state as a vector, without choosing a position, momentum, or some other basis for the vectors.

The eigenvectors of any Hermetian operator form a complete, orthonormal basis,

$$\hat{O}\,|\lambda\rangle = \lambda\,|\lambda\rangle$$

and Hermitian operators correspond to dynamical variables – the phyical quantitites we wish to measure. This lets us define bases of position, momentum or energy eigenkets, though many more are possible.

1 Position basis

The most familiar basis is the position basis. Since we can measure position vectors, we have a vector of Hermitian position operators, $\hat{\mathbf{X}} = \left(\hat{X}, \hat{Y}, \hat{Z}\right) \Leftrightarrow \hat{X}_i$, $\hat{\mathbf{X}}^\dagger = \hat{\mathbf{X}}$, with continuous eigenvalues, $\mathbf{x}$, giving the position vector of a particle:

$$\hat{\mathbf{X}}\,|\mathbf{x}\rangle = \mathbf{x}\,|\mathbf{x}\rangle$$

When expanded in the position basis, the components comprise the familiar wave function. To expand a state $|\psi\rangle$ in a position basis, we use the position eigenbra, $\langle\mathbf{x}|$, to get

$$\langle\mathbf{x}\,|\psi\rangle$$

This is just a complex number for each position vector $\mathbf{x}$, i.e., a function, $\psi(\mathbf{x})$. Normalization of the wave function may be written as

$$1 = \langle\psi|\,\psi\rangle$$

$$
\begin{aligned}
&= \langle\psi|\,\hat{1}\,|\psi\rangle \\
&= \int d^3x\,\langle\psi|\,\mathbf{x}\rangle\,\langle\mathbf{x}|\,\psi\rangle \\
&= \int d^3x\;\psi^*(\mathbf{x})\,\psi(\mathbf{x})
\end{aligned}
$$

so we recover our usual rule with $\psi^*(\mathbf{x})\,\psi(\mathbf{x})$ as the probability density.

Measurements in the x, y and z directions commute:

$$\left[\hat{X}_i, \hat{X}_j\right] = 0$$

so that all three eigenvalues may be specified at once.

This is a general property. Suppose we have a set of basis states which are simultaneous eigenkets, $|\alpha,\beta\rangle$ of two different Hermitian dynamical variables $\hat{A}, \hat{B}$, that is

$$
\begin{aligned}
\hat{A}\,|\alpha,\beta\rangle &= \alpha\,|\alpha,\beta\rangle \\
\hat{B}\,|\alpha,\beta\rangle &= \beta\,|\alpha,\beta\rangle
\end{aligned}
$$

Then the commutator acting on the basis gives

$$
\begin{aligned}
\left[\hat{A},\hat{B}\right]|\alpha,\beta\rangle &= \left(\hat{A}\hat{B}-\hat{B}\hat{A}\right)|\alpha,\beta\rangle \\
&= \hat{A}\hat{B}\,|\alpha,\beta\rangle - \hat{B}\hat{A}\,|\alpha,\beta\rangle \\
&= \hat{A}\beta\,|\alpha,\beta\rangle - \hat{B}\alpha\,|\alpha,\beta\rangle \\
&= \beta\hat{A}\,|\alpha,\beta\rangle - \alpha\hat{B}\,|\alpha,\beta\rangle \\
&= (\beta\alpha-\alpha\beta)\,|\alpha,\beta\rangle \\
&= 0
\end{aligned}
$$

so the action of the commutator on any basis ket gives zero. Therefore, since the basis is complete, we may write *any* state as a superposition,

$$|\psi\rangle = \iint d\alpha d\beta A(\alpha,\beta)\,|\alpha,\beta\rangle$$

Then we have

$$
\begin{aligned}
\left[\hat{A},\hat{B}\right]|\psi\rangle &= \left[\hat{A},\hat{B}\right]\iint d\alpha d\beta A(\alpha,\beta)\,|\alpha,\beta\rangle \\
&= \iint d\alpha d\beta A(\alpha,\beta)\left[\hat{A},\hat{B}\right]|\alpha,\beta\rangle \\
&= 0
\end{aligned}
$$

Since $\left[\hat{A},\hat{B}\right]$ vanishes acting on *every* state, it is the zero operator,

$$\left[\hat{A},\hat{B}\right] = 0$$

Conversely, suppose $\left[\hat{A},\hat{B}\right]$ is not zero. Then there exists some state such that

$$\left[\hat{A},\hat{B}\right]|\psi\rangle \neq 0$$

and the existence of simultaneous eigenkets is a contradiction. Therefore, there exists a basis of eigenstates of two operators at once if and only if those operators commute. This gives us, at least in principle, a way to label states. If we can find a maximal set of mutually commuting operators, then we may label all states by their eigenvalues.

2 Momentum basis

We also know that momentum is a dynamical variable (an "observable"). Therefore, there is a Hermitian operator

$$\begin{aligned}\hat{\mathbf{P}} &= \hat{\mathbf{P}}^{\dagger} \\ \hat{\mathbf{P}} &= \left(\hat{P}_x, \hat{P}_y, \hat{P}_z\right) = \hat{P}_i\end{aligned}$$

with eigenstates, $|\mathbf{p}\rangle$, satisfying

$$\hat{\mathbf{P}} |\mathbf{p}\rangle = \mathbf{p} |\mathbf{p}\rangle$$

We would like to find the form of this operator in a position basis.

In a finite basis, finding the form of an operator means finding the matrix elements. Thus, for the spin operator $\hat{S}_x$, knowing the matrix

$$\begin{pmatrix} \langle +| \hat{S}_x |+\rangle & \langle +| \hat{S}_x |-\rangle \\ \langle -| \hat{S}_x |+\rangle & \langle -| \hat{S}_x |-\rangle \end{pmatrix}$$

gives the form of the operator in the z-basis. The situation is completely analogous in a continuous basis: we seek the matrix elements $\langle \mathbf{x}'| \hat{\mathbf{P}} |\mathbf{x}"\rangle$.

We begin by letting the momentum operator $\hat{\mathbf{P}}$ act on a plane wave state of wave number $\mathbf{k}$, $\langle \mathbf{x}| \psi\rangle = Ae^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}$. Inserting an identity operator,

$$\begin{aligned}\hat{\mathbf{P}} |\psi\rangle &= \hat{\mathbf{P}} \left(\int d^3x\, |\mathbf{x}\rangle \langle \mathbf{x}|\right) |\psi\rangle \\ &= \hat{\mathbf{P}} \int d^3x\, |\mathbf{x}\rangle \langle \mathbf{x}| \psi\rangle \\ &= \hat{\mathbf{P}} \int d^3x\; Ae^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)} |\mathbf{x}\rangle\end{aligned}$$

We know that for a plane wave the result must be the momentum, $\mathbf{p} = \hbar\mathbf{k}$, so

$$\hbar\mathbf{k} |\psi\rangle = \int d^3x\; Ae^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)} \hat{\mathbf{P}} |\mathbf{x}\rangle$$

Now look at this vector equation in a position basis (or, look at the $|\mathbf{x}'\rangle$ component of this vector). Placing the $\langle \mathbf{x}'|$ bra on the left,

$$\begin{aligned}\langle \mathbf{x}'| \hbar\mathbf{k} |\psi\rangle &= \int d^3x\; Ae^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)} \langle \mathbf{x}'| \hat{\mathbf{P}} |\mathbf{x}\rangle \\ \hbar\mathbf{k}\psi(\mathbf{x}') &= \int d^3x\; Ae^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)} \langle \mathbf{x}'| \hat{\mathbf{P}} |\mathbf{x}\rangle \\ \hbar\mathbf{k}Ae^{i\left(\mathbf{k}\cdot\mathbf{x}'-\omega t\right)} &= \int d^3x\; Ae^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)} \langle \mathbf{x}'| \hat{\mathbf{P}} |\mathbf{x}\rangle \\ \hbar\mathbf{k}Ae^{i\mathbf{k}\cdot\mathbf{x}'} &= \int d^3x\; Ae^{i\mathbf{k}\cdot\mathbf{x}} \langle \mathbf{x}'| \hat{\mathbf{P}} |\mathbf{x}\rangle\end{aligned}$$

The integral on the right is just the Fourier transform of the matrix element we want. All we need to do is take the inverse transform of both sides. Multiply by $e^{-i\mathbf{k}\cdot\mathbf{x}"}$ and integrate over d^3k,

$$\begin{aligned}\hbar\mathbf{k}Ae^{i\mathbf{k}\cdot\mathbf{x}'} &= \int d^3x\; Ae^{i\mathbf{k}\cdot\mathbf{x}} \langle \mathbf{x}'| \hat{\mathbf{P}} |\mathbf{x}\rangle \\ \int d^3k\; \hbar\mathbf{k}Ae^{i\mathbf{k}\cdot\mathbf{x}'}e^{-i\mathbf{k}\cdot\mathbf{x}"} &= \int d^3k \int d^3x\; Ae^{i\mathbf{k}\cdot\mathbf{x}}e^{-i\mathbf{k}\cdot\mathbf{x}"} \langle \mathbf{x}'| \hat{\mathbf{P}} |\mathbf{x}\rangle\end{aligned}$$

$$\begin{aligned}
\int d^3k\ \hbar\mathbf{k}e^{i\mathbf{k}\cdot\left(\mathbf{x}'-\mathbf{x}"\right)} &= \int d^3x\ \left\langle\mathbf{x}'\right|\hat{\mathbf{P}}\left|\mathbf{x}\right\rangle\int d^3k\ e^{i\mathbf{k}\cdot\left(\mathbf{x}'-\mathbf{x}"\right)} \\
\int d^3k\ \hbar\mathbf{k}e^{i\mathbf{k}\cdot\left(\mathbf{x}'-\mathbf{x}"\right)} &= \int d^3x\ \left\langle\mathbf{x}'\right|\hat{\mathbf{P}}\left|\mathbf{x}\right\rangle(2\pi)^3\,\delta^3\left(\mathbf{x}'-\mathbf{x}"\right) \\
\int d^3k\ \hbar\mathbf{k}e^{i\mathbf{k}\cdot\left(\mathbf{x}'-\mathbf{x}"\right)} &= (2\pi)^3\left\langle\mathbf{x}'\right|\hat{\mathbf{P}}\left|\mathbf{x}"\right\rangle
\end{aligned}$$

Now notice that we may evaluate the left hand side using a derivative,

$$\begin{aligned}
\int d^3k\ \hbar\mathbf{k}e^{i\mathbf{k}\cdot\left(\mathbf{x}'-\mathbf{x}"\right)} &= \int d^3k\ \hbar\left(i\boldsymbol{\nabla}_{x"}\right)e^{i\mathbf{k}\cdot\left(\mathbf{x}'-\mathbf{x}"\right)} \\
&= \hbar\left(i\boldsymbol{\nabla}_{x"}\right)\int d^3k\ e^{i\mathbf{k}\cdot\left(\mathbf{x}'-\mathbf{x}"\right)} \\
&= (2\pi)^3\,i\hbar\boldsymbol{\nabla}_{x"}\delta^3\left(\mathbf{x}'-\mathbf{x}"\right)
\end{aligned}$$

Equating the two results, we have the matrix elements of the momentum operator in the position basis:

$$\left\langle\mathbf{x}'\right|\hat{\mathbf{P}}\left|\mathbf{x}"\right\rangle = i\hbar\boldsymbol{\nabla}_{x"}\delta^3\left(\mathbf{x}'-\mathbf{x}"\right)$$

To see how this works, we let $\hat{\mathbf{P}}$ act on a general state, $\hat{\mathbf{P}}\left|\psi\right\rangle$ and insert an identity operator,

$$\hat{\mathbf{P}}\left|\psi\right\rangle = \hat{\mathbf{P}}\int d^3x\left|\mathbf{x}\right\rangle\left\langle\mathbf{x}\right|\left.\psi\right\rangle$$

Now, in a position basis,

$$\begin{aligned}
\left\langle\mathbf{x}'\right|\hat{\mathbf{P}}\left|\psi\right\rangle &= \int d^3x\left\langle\mathbf{x}'\right|\hat{\mathbf{P}}\left|\mathbf{x}\right\rangle\left\langle\mathbf{x}\right|\left.\psi\right\rangle \\
&= \int d^3x\left(i\hbar\boldsymbol{\nabla}_x\delta^3\left(\mathbf{x}'-\mathbf{x}\right)\right)\psi\left(\mathbf{x}\right)
\end{aligned}$$

Integrate by parts,

$$\begin{aligned}
\left\langle\mathbf{x}'\right|\hat{\mathbf{P}}\left|\psi\right\rangle &= \int d^3x\boldsymbol{\nabla}_x\left(i\hbar\delta^3\left(\mathbf{x}'-\mathbf{x}\right)\psi\left(\mathbf{x}\right)\right) - \int d^3x\left(i\hbar\delta^3\left(\mathbf{x}'-\mathbf{x}\right)\boldsymbol{\nabla}_x\psi\left(\mathbf{x}\right)\right) \\
&= -i\hbar\int d^3x\left(\delta^3\left(\mathbf{x}'-\mathbf{x}\right)\boldsymbol{\nabla}_x\psi\left(\mathbf{x}\right)\right) \\
&= -i\hbar\boldsymbol{\nabla}_{x'}\psi\left(\mathbf{x}'\right)
\end{aligned}$$

This is the form of the momentum operator which we intuited in deriving the Schrödinger equation. Notice that the first integral vanishes because the delta function vanishes away from $\mathbf{x}'=\mathbf{x}$, or equivalently because the wave function vanishes at infinity.

3 Change of basis

Suppose we are given a state in the momentum basis, $\left\langle\mathbf{p}\right|\left.\psi\right\rangle$, and wish to find it in the position basis, $\left\langle\mathbf{x}\right|\left.\psi\right\rangle = \psi\left(\mathbf{x}\right)$. We write what we are after and insert the indentity operator in the momentum basis,

$$\begin{aligned}
\psi\left(\mathbf{x}\right) &= \left\langle\mathbf{x}\right|\left.\psi\right\rangle \\
&= \int d^3p\left\langle\mathbf{x}\right|\left.\mathbf{p}\right\rangle\left\langle\mathbf{p}\right|\left.\psi\right\rangle
\end{aligned}$$

We need the numbers $\langle \mathbf{x} | \mathbf{p} \rangle$ to complete the integral. These are the components of a unitary matrix, since the product of $M = \langle \mathbf{x} | \mathbf{p} \rangle$ with its adjoint $M^\dagger = \langle \mathbf{p} | \mathbf{x} \rangle$ is

$$\begin{aligned} M^\dagger M &= \int d^3x \, \langle \mathbf{p} | \mathbf{x} \rangle \langle \mathbf{x} | \mathbf{p}' \rangle \\ &= \langle \mathbf{p} | \mathbf{p}' \rangle \\ &= \delta^3 (\mathbf{p} - \mathbf{p}') \\ &= \mathbf{1} \end{aligned}$$

It is a unitary transformation that takes us from one basis to another. This is important, since it preserves Hermiticity,

$$\hat{\tilde{H}} = U \hat{H} U^\dagger$$

implies

$$\begin{aligned} \hat{\tilde{H}}^\dagger &= \left(U \hat{H} U^\dagger \right)^\dagger \\ &= U^{\dagger\dagger} \hat{H}^\dagger U^\dagger \\ &= U \hat{H} U^\dagger \end{aligned}$$

These matrix elements $\langle \mathbf{x} | \mathbf{p} \rangle$ are found as follows. Projecting $\mathbf{p} | \mathbf{p} \rangle = \hat{\mathbf{P}} | \mathbf{p} \rangle$ with $\langle \mathbf{x} |$, and inserting an identity, we have

$$\begin{aligned} \mathbf{p} \langle \mathbf{x} | \mathbf{p} \rangle &= \langle \mathbf{x} | \hat{\mathbf{P}} | \mathbf{p} \rangle \\ &= \int d^3x' \, \langle \mathbf{x} | \hat{\mathbf{P}} | \mathbf{x}' \rangle \langle \mathbf{x}' | \mathbf{p} \rangle \\ &= \int d^3x' \, \left(i\hbar \boldsymbol{\nabla}_{x'} \delta^3 (\mathbf{x} - \mathbf{x}') \right) \langle \mathbf{x}' | \mathbf{p} \rangle \\ &= -i\hbar \int d^3x' \, \delta^3 (\mathbf{x} - \mathbf{x}') \boldsymbol{\nabla}_{x'} \langle \mathbf{x}' | \mathbf{p} \rangle \\ &= -i\hbar \boldsymbol{\nabla}_x \langle \mathbf{x} | \mathbf{p} \rangle \end{aligned}$$

This is a simple differential equation for the inner product,

$$\mathbf{p} \langle \mathbf{x} | \mathbf{p} \rangle = -i\hbar \boldsymbol{\nabla}_x \langle \mathbf{x} | \mathbf{p} \rangle$$

with the solution

$$\langle \mathbf{x} | \mathbf{p} \rangle = A e^{\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{x}}$$

The normalization constant A may be found from

$$\begin{aligned} \delta^3 (\mathbf{x} - \mathbf{x}') &= \langle \mathbf{x} | \mathbf{x}' \rangle \\ &= \int d^3p \, \langle \mathbf{x} | \mathbf{p} \rangle \langle \mathbf{p} | \mathbf{x}' \rangle \\ &= \int d^3p \, A e^{\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{x}} A^* e^{-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{x}'} \\ &= A^* A \int d^3p \, e^{\frac{i}{\hbar} \mathbf{p} \cdot (\mathbf{x} - \mathbf{x}')} \\ &= A^* A \hbar^3 \int d^3k \, e^{i \mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')} \\ &= A^* A \hbar^3 (2\pi)^3 \delta^3 (\mathbf{x} - \mathbf{x}') \end{aligned}$$

Choose the normalization real gives

$$\langle \mathbf{x} | \, \mathbf{p} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}}$$

Thus, the transition functions between the position and momentum bases are just Fourier modes.