Quantum One
Canonical Commutation Relations
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We begin the current segment by deriving what are referred to as canonical commutation relations.
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This extends to the operator $Z$ as well, so we can generally write

$$[X_i, X_j] = 0$$
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Subtracting these two terms, we find that in the position representation
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\[ \langle \vec{r} | [X_i, K_j] \psi \rangle = -i x_i \frac{\partial \psi}{\partial x_j} + i \{ \delta_{ij} \psi (\vec{r}) + x_i \frac{\partial \psi}{\partial x_j} \} \]
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which often appears in terms of the momentum operator, in the form first obtained by Max Born, i.e.,

\[ [X_i, P_j] = i\hbar\delta_{ij} \]
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Changing Representations: Unitary Operators
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In fact, given any two ONBs for \( S \), there exists a unitary operator \( U \) that maps one set onto another, and whose adjoint maps the second set back onto the first.
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From these expansion coefficients, we can construct a ket-bra expansion for $U$.

$$U = \sum_{i,j} |\psi_i\rangle U_{i,j} \langle \psi_j| = \sum_{i,j} |\psi_i\rangle \langle \psi_i | \phi_j \rangle \langle \psi_j|$$
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Identifying the identity operator on the left, this reduces to a single sum

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The **practical use** of these matrix elements come when we wish to **transform from one representation to another**.
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The practical use of these matrix elements come when we wish to **transform from one representation to another**.

Suppose, for example, that you and I have both solved a given problem using **different representations**, and we want to **compare** our results.
In addition, we note that

\[ U_{ij}^+ = \langle \phi_i | U^+ | \phi_j \rangle = \langle \phi_i | \psi_j \rangle \]

are just the expansion coefficients for the basis states \( \{ | \psi_i \rangle \} \) in terms of the basis states \( \{ | \phi_i \rangle \} \). So we have a related pair of relations involving the matrix elements of \( U \) and \( U^+ \), i.e.,

\[ U_{ij} = \langle \psi_i | \phi_j \rangle \]
\[ U_{ij}^+ = \langle \phi_i | \psi_j \rangle \]

The **practical use** of these matrix elements come when we wish to **transform from one representation to another**.

Suppose, for example, that you and I have both solved a given problem using **different representations**, and we want to **compare** our results.

Then I need to transform expressions derived in my representation to those derived in yours, and vice versa.
Transformation of Kets - Let $|\chi\rangle$ be an arbitrary ket in the space.
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This last relation, thus takes the form

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which is equivalent to a matrix-column vector multiplication, i.e.,

\[
\begin{pmatrix}
\chi_1 \\
\chi_2 \\
\vdots
\end{pmatrix}
= 
\begin{pmatrix}
U_{11} & U_{12} & \cdots \\
U_{21} & U_{22} & \cdots \\
\vdots & \vdots & \ddots
\end{pmatrix}
\begin{pmatrix}
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\[ \psi_i \rightarrow \phi_i \]
Transformation of Kets

By a similar approach it can be shown that the reverse transformation is effected by the matrix representing $U^+$. Thus, we have the relation

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$\phi_i \rightarrow \psi_i$
Transformation of Matrices - If $A$ is an operator it has matrix elements in the two bases considered above of the form

$$A_{ij} = \langle \psi_i | A | \psi_j \rangle \rightarrow [A]$$
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To find the relationship between the matrices representing this operator in these two different bases we write

$$A_{ij} = \langle \psi_i | 1 A 1 | \psi_j \rangle$$
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which can be expressed as a threefold matrix product

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The reverse transformation is found in the same way, and yields the result

$$[A'] = [U^+] [A] [U]$$
Transformation of Representations: Extension to Continuous Representations

Let $|\psi\rangle$ be an arbitrary vector in the space of a quantum particle in three dimensions, i.e., the space spanned by the vectors $|\vec{r}\rangle$ of the position representation and by the vectors $|\vec{k}\rangle$ of the wavevector representation.
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Let $|\psi\rangle$ be an arbitrary vector in the space of a quantum particle in three dimensions, i.e., the space spanned by the vectors $|\vec{r}\rangle$ of the position representation and by the vectors $|\vec{k}\rangle$ of the wavevector representation.

We can expand the ket $|\psi\rangle$ in either of these two bases, i.e.,

$$|\psi\rangle = \int d^3 r \, \psi(\vec{r}) \, |\vec{r}\rangle$$
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(Let’s pretend we didn’t already know...)
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We can find out in the same way as we just did for the discrete case, i.e., we write

$$\psi(\vec{r}) = \langle \vec{r} | \psi \rangle = \langle \vec{r} | \mathbf{1} | \psi \rangle = \int d^3k \; \langle \vec{r} | \vec{k} \rangle \langle \vec{k} | \psi \rangle$$
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which we (suggestively) write as

\[ \psi(\vec{r}) = \int d^3 k \ U(\vec{r}, \vec{k}) \psi(\vec{k}) \]
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which we (suggestively) write as

$$\psi(\vec{r}) = \int d^3k \ U(\vec{r}, \vec{k}) \psi(\vec{k})$$

where the (continuous) matrix elements of the unitary operator connecting these two bases are

$$U(\vec{r}, \vec{k}) = \langle \vec{r} | \vec{k} \rangle = \frac{e^{i\vec{k} \cdot \vec{r}}}{(2\pi)^{3/2}}$$
Transformation of Representations: Extension to Continuous Representations

Thus, we find that

\[ \psi(\vec{r}) = \int d^3 k \frac{e^{i\vec{k} \cdot \vec{r}}}{(2\pi)^{3/2}} \psi(\vec{k}) \]

which, of course, we already knew.
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which, of course, we already knew. Similarly, we find that

\[ \psi(\vec{k}) = \int d^3 r \ U^+(\vec{k}, \vec{r}) \psi(\vec{r}) = \int d^3 r \ \frac{e^{-i\vec{k} \cdot \vec{r}}}{(2\pi)^{3/2}} \psi(\vec{r}) \]
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Thus, the Fourier transform is just an example of a unitary transformation from one continuous basis to another.

It is also possible to use the unitary transformation represented by the Fourier transform to derive the matrix elements of some of the operators we have already encountered.
Transformation of Representations: Extension to Continuous Representations

As an example, consider the position operator \( \vec{R} \) whose matrix elements in the position representation are given by the expression

\[
\langle \vec{r} | \vec{R} | \vec{r}' \rangle = \vec{R}(\vec{r}, \vec{r}') = \vec{r} \delta(\vec{r} - \vec{r}')
\]
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$$\vec{R}(\vec{k}, \vec{k}') = \int d^3r \int d^3k' \ U^+(\vec{k}, \vec{r}) \ \vec{R}(\vec{r}, \vec{r}') \ U(\vec{r}', \vec{k})$$
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\[
\vec{R}(\vec{k}, \vec{k}') = \int d^3r \int d^3r' U^+(\vec{k}, \vec{r}) \vec{R}(\vec{r}, \vec{r}') U(\vec{r}', \vec{k}) = \frac{1}{(2\pi)^3} \int d^3r \int d^3r' e^{-i\vec{k} \cdot \vec{r}} \vec{r} \delta(\vec{r} - \vec{r}') e^{i\vec{k}' \cdot \vec{r}'}
\]
Transformation of Representations: Extension to Continuous Representations

As an example, consider the position operator $\hat{R}$ whose matrix elements in the position representation are given by the expression

$$\langle \vec{r} | \hat{R} | \vec{r}' \rangle = \hat{R}(\vec{r}, \vec{r}') = \vec{r} \delta(\vec{r} - \vec{r}')$$

The matrix elements in the wavevector representation can be obtained from this by a unitary transformation, i.e.,

\[
\begin{align*}
\hat{R}(\vec{k}, \vec{k}') &= \int d^3r \int d^3r' U^+(\vec{k}, \vec{r}) \hat{R}(\vec{r}, \vec{r}') U(\vec{r}', \vec{k}) \\
&= \frac{1}{(2\pi)^3} \int d^3r \int d^3r' e^{-i\vec{k}\cdot\vec{r}} \vec{r} \delta(\vec{r} - \vec{r}') e^{i\vec{k}'\cdot\vec{r}'} \\
&= \frac{1}{(2\pi)^3} \int d^3r \vec{r} e^{-i(\vec{k} - \vec{k}')\cdot\vec{r}}
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$$= \frac{1}{(2\pi)^3} \int d^3r \int d^3r' \ e^{-i\vec{k} \cdot \vec{r}} \ \vec{r} \delta(\vec{r} - \vec{r}') \ e^{i\vec{k}' \cdot \vec{r}' }$$

$$= \frac{1}{(2\pi)^3} \int d^3r \ e^{-i(\vec{k} - \vec{k}') \cdot \vec{r}} = i \vec{\nabla}_k \left[ \int \frac{d^3r}{(2\pi)^3} \ e^{i(\vec{k} - \vec{k}') \cdot \vec{r}} \right]$$
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We saw how to transform between two discrete representations, using the matrices that represent the unitary operators connecting them, and extended this idea to continuous representation, noting that the Fourier transform relation between position and momentum actually represents a unitary transformation between those two representations.
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In the next segment we learn about a number of properties that the matrices that represent a given linear operator share, i.e., representation independent properties.