CHANGE OF BASIS

Transformation Operator

Suppose we have two incompatible observables A and B. The ket space in question can be viewed as being spanned either by the set {|a'>} or by the set {|b'>}.

Our basic task is to construct a transformation operator that connects the old orthonormal set {|a'>} and the new orthonormal set {|b'>}.

To this end, we first show the following:

Theorem. Given two sets of base kets, both satisfying orthonormality and completeness, there exists a unitary operator U such that

$$|b^{(1)}\rangle = U|a^{(1)}\rangle, |b^{(2)}\rangle = U|a^{(2)}\rangle, \ldots, |b^{(N)}\rangle = U|a^{(N)}\rangle$$

Proof. We prove this theorem by explicit construction. We assert that the following operator will do the job:

$$U = \sum_k |b^{(k)}\rangle\langle a^{(k)}| \Rightarrow U|a^{(l)}\rangle = |b^{(l)}\rangle \checkmark$$

$$U^\dagger U = \sum_k \sum_l |a^{(l)}\rangle\langle b^{(l)}|b^{(k)}\rangle\langle a^{(k)}| = \sum_k |a^{(k)}\rangle\langle a^{(k)}| = 1 \checkmark$$

Transformation Matrix

$$U = \sum_k |b^{(k)}\rangle\langle a^{(k)}|$$

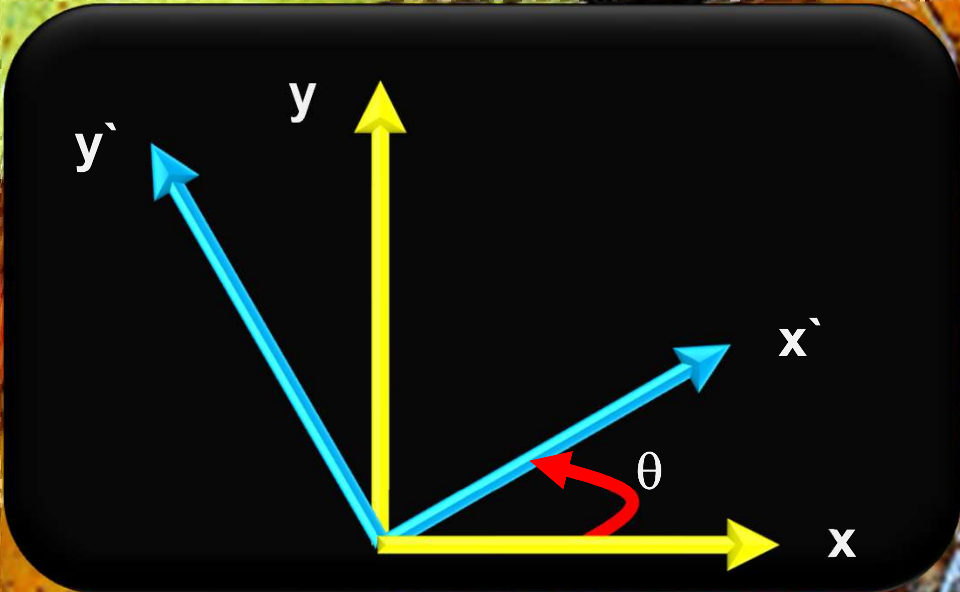
$$U|a^{(l)}\rangle = |b^{(l)}\rangle$$

$$\langle a^{(k)}|U|a^{(l)}\rangle = \langle a^{(k)}|b^{(l)}\rangle$$

In other words, the matrix elements of the U operator are built up of the inner products of old base bras and new base kets.

The square matrix made up of $<a^{(k)})|U|a^{(l)})$ is referred to as the transformation matrix from the $\{|a'>\}$ basis to the $\{|b'>\}$ basis.

We recall that the rotation matrix in three dimensions that changes one set of unit base vectors (**x, y, z**) into another set (**x', y', z'**) can be written as:



$$R = \begin{pmatrix} \hat{\mathbf{x}}\cdot\hat{\mathbf{x}}' & \hat{\mathbf{x}}\cdot\hat{\mathbf{y}}' & \hat{\mathbf{x}}\cdot\hat{\mathbf{z}}' \\ \hat{\mathbf{y}}\cdot\hat{\mathbf{x}}' & \hat{\mathbf{y}}\cdot\hat{\mathbf{y}}' & \hat{\mathbf{y}}\cdot\hat{\mathbf{z}}' \\ \hat{\mathbf{z}}\cdot\hat{\mathbf{x}}' & \hat{\mathbf{z}}\cdot\hat{\mathbf{y}}' & \hat{\mathbf{z}}\cdot\hat{\mathbf{z}}' \end{pmatrix}$$

$$\hat{\mathbf{x}}' = \hat{\mathbf{x}}\cos\theta + \hat{\mathbf{y}}\sin\theta$$

$$\hat{\mathbf{y}}' = -\hat{\mathbf{x}}\sin\theta + \hat{\mathbf{y}}\cos\theta$$

$$\hat{\mathbf{x}}.\hat{\mathbf{x}}' = \cos\theta \qquad \hat{\mathbf{x}}.\hat{\mathbf{y}}' = -\sin\theta$$

$$\hat{\mathbf{y}}.\hat{\mathbf{x}}' = \sin\theta \qquad \hat{\mathbf{y}}.\hat{\mathbf{y}}' = \cos\theta$$

$$\mathbf{R} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

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Given an arbitrary ket |α> whose expansion coefficients <a'|α> are known in the old basis, how can we obtain <b'|α>, the expansion coefficients in the new basis?

$$|\alpha\rangle = \sum_l |a^{(l)}\rangle\langle a^{(l)}|\alpha\rangle$$

$$(\text{New}) = (U^\dagger)(\text{old})$$

$$\langle b^{(k)}|\alpha\rangle = \sum_l \langle b^{(k)}|a^{(l)}\rangle\langle a^{(l)}|\alpha\rangle = \sum_l \langle a^{(k)}|U^\dagger|a^{(l)}\rangle\langle a^{(l)}|\alpha\rangle$$

$$U|a^{(l)}\rangle = |b^{(l)}\rangle$$

$$< a^{(l)} | U^\dagger =< b^{(l)} |$$

In matrix notation, it states that the column matrix for |α> in the new basis can be obtained just by applying the square matrix U^+ to the column matrix in the old basis:

The relationships between the old matrix elements and the new matrix elements are also easy to obtain:

$$\langle b^{(k)}|X|b^{(l)}\rangle = \sum_m \sum_n \langle b^{(k)}|a^{(m)}\rangle\langle a^{(m)}|X|a^{(n)}\rangle\langle a^{(n)}|b^{(l)}\rangle$$

$$= \sum_m \sum_n \langle a^{(k)}|U^\dagger|a^{(m)}\rangle\langle a^{(m)}|X|a^{(n)}\rangle\langle a^{(n)}|U|a^{(l)}\rangle$$

This is simply the well-known formula for a similarity transformation in matrix algebra,

$$X' = U^\dagger X U$$

The trace of an operator X is defined as the sum of diagonal elements:

$$\mathrm{tr}(X) = \sum_{a'} \langle a'|X|a'\rangle$$

The trace of an operator X is independent of representation:

$$\sum_{a'} \langle a'|X|a'\rangle = \sum_{a'}\sum_{b'}\sum_{b''} \langle a'|b'\rangle\langle b'|X|b''\rangle\langle b''|a'\rangle$$

$$= \sum_{b'}\sum_{b''} \langle b''|b'\rangle\langle b'|X|b''\rangle = \sum_{b'} \langle b'|X|b'\rangle \checkmark$$

We can also prove that

$$\mathrm{tr}(XY) = \mathrm{tr}(YX)$$

$$\mathrm{tr}(XY) = \sum_{a'} < a' | XY | a' >$$

$$= \sum_{a'b'} < a' | X | b' >< b' | Y | a' >$$

$$= \sum_{a'b'} < b' | Y | a' >< a' | X | b' >$$

$$= \sum_{b'} < b' | YX | b' >$$

$$= \sum_{a'} < a' | YX | a' > = \mathrm{tr}(YX) \checkmark$$

$$\mathrm{tr}(U^{\dagger}XU) = \mathrm{tr}(X)$$

$$\mathrm{tr}(U^{\dagger}XU) = \sum_{a'} \langle a' | U^{\dagger}XU | a' \rangle$$

$$= \sum_{a'b'b''} \langle a' | U^{\dagger} | b' \rangle \langle b' | X | b'' \rangle \langle b'' | U | a' \rangle$$

$$= \sum_{a'b'b''} \langle b'' | U | a' \rangle \langle a' | U^{\dagger} | b' \rangle \langle b' | X | b'' \rangle$$

$$= \sum_{b'b''} \langle b'' | U^{\dagger}U | b' \rangle \langle b' | X | b'' \rangle$$

$$= \sum_{b'b''} \langle b'' | b' \rangle \langle b' | X | b'' \rangle \qquad = \sum_{b'} \langle b' | X | b' \rangle = \mathrm{tr}(X)$$

$$\mathbf{tr}\big(|a'\rangle\langle a''|\big) = \delta_{a'a''}$$

$$\mathrm{tr}(|a'><a''|) = \sum_{b'} <b'|a'><a''|b'> = <a''|a'> = \delta_{a'a''}$$

$$\mathbf{tr}\big(|b'\rangle\langle a'|\big) = \langle a'|b'\rangle$$

$$\mathrm{tr}(|b'><a'|) = \sum_{c'} <c'|b'><a'|c'> = \sum_{c'} <a'|c'><c'|b'>$$

$$= <a'|b'>$$

In summery we have

$$\mathrm{tr}(XY) = \mathrm{tr}(YX)$$

$$\mathrm{tr}(U^\dagger XU) = \mathrm{tr}(X)$$

$$\mathrm{tr}(|a'\rangle\langle a''|) = \delta_{a'a''}$$

$$\mathrm{tr}(|b'\rangle\langle a'|) = \langle a'|b'\rangle$$

Diagonalization

$$B|b'\rangle = b'|b'\rangle$$

$$\sum_{a'} \langle a''|B|a'\rangle\langle a'|b'\rangle = b'\langle a''|b'\rangle$$

$$\begin{pmatrix} B_{11} & B_{12} & B_{13} & \cdots \\ B_{21} & B_{22} & B_{23} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} C_1^{(l)} \\ C_2^{(l)} \\ \vdots \end{pmatrix} = b^{(l)} \begin{pmatrix} C_1^{(l)} \\ C_2^{(l)} \\ \vdots \end{pmatrix}$$

$$B_{ij} = \langle a^{(i)}|B|a^{(j)}\rangle$$

$$C_k^{(l)} = \langle a^{(k)}|b^{(l)}\rangle$$

$$\det(B - \lambda 1) = 0$$

For diagonalization procedure the Hermiticity of B is important.

For example, S_+ operator which is obviously non-Hermitian cannot be diagonalized by any unitary matrix.

$$S_+ \doteq \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

The eigenkets of a non-Hermitian operator are known not to form a complete orthonormal set, and the formalism we have developed in this section cannot be immediately applied.

Unitary Equivalent Observables

Theorem. Consider again two sets of orthonormal basis {|a'>} and {|b'>} connected by the U operator. Knowing U, we may construct a unitary transform of A, UAU^{-1}; then A and UAU^{-1} are said to be unitary equivalent observables.

$$U = \sum_k |b^{(k)}\rangle\langle a^{(k)}|$$

$$U|a^{(l)}\rangle = |b^{(l)}\rangle$$

$$A|a^{(l)}\rangle = a^{(l)}|a^{(l)}\rangle$$

$$UAU^{-1}U|a^{(l)}\rangle = a^{(l)}U|a^{(l)}\rangle$$

$$(UAU^{-1})|b^{(l)}\rangle = a^{(l)}|b^{(l)}\rangle$$

This deceptively simple result is quite profound.

$$A|a^{(l)}\rangle = a^{(l)}|a^{(l)}\rangle$$

$$(UAU^{-1})|b^{(l)}\rangle = a^{(l)}|b^{(l)}\rangle$$

It tells us that the |b`>'s are eigenkets of UAU^{-1} with exactly the same eigenvalues as the A eigenvalues.

In other words, unitary equivalent observables have identical spectra.

$$B|b^{(l)}\rangle = b^{(l)}|b^{(l)}\rangle$$

$$(UAU^{-1})|b^{(l)}\rangle = a^{(l)}|b^{(l)}\rangle$$

we infer that B and UAU^{-1} are simultaneously diagonalizable.

Is UAU^{-1} the same as B itself?

The answer quite often is yes in cases of physical interest.

Take, for example, Sx and Sz.

They are related by a unitary operator, which is actually the rotation operator around the y-axis by angle $\pi/2$.

In this case Sx itself is the unitary transform of Sz.

we know that Sx and Sz exhibit the same set of eigenvalues—namely, $+\hbar/2$ and $-\hbar/2$—we see that our theorem holds in this particular example.

Continuous Spectra

The observables considered so far have all been assumed to exhibit discrete eigenvalue spectra. In quantum mechanics, however, there are observables with continuous eigenvalues.

$$\langle a'|a''\rangle = \delta_{a'a''} \;\Rightarrow\; \langle \xi'|\xi''\rangle = \delta(\xi' - \xi'')$$

$$\sum_{a'} |a'\rangle\langle a'| = 1 \;\Rightarrow\; \int d\xi' |\xi'\rangle\langle \xi'| = 1$$

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \;\Rightarrow\; |\alpha\rangle = \int d\xi' |\xi'\rangle\langle \xi'|\alpha\rangle$$

$$\sum_{a'} |\langle a'|\alpha\rangle|^2 = 1 \;\Rightarrow\; \int d\xi' |\langle \xi'|\alpha\rangle|^2 = 1$$

$$\langle \beta|\alpha\rangle = \sum_{a'} \langle \beta|a'\rangle\langle a'|\alpha\rangle \;\Rightarrow\; \langle \beta|\alpha\rangle = \int d\xi' \langle \beta|\xi'\rangle\langle \xi'|\alpha\rangle$$

$$\langle a''|A|a'\rangle = a'\delta_{a'a''} \;\Rightarrow\; \langle \xi''|\xi|\xi'\rangle = \xi'\delta(\xi'' - \xi')$$

Position Eigenkets and Position Measurements

$$x|x'\rangle = x'|x'\rangle$$

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

Measurement or Filtering

$|x'>$

$$|\mathbf{x}'\rangle \equiv |x', y', z'\rangle$$

The probability of finding the particle in x` to x`+dx`

$$|\langle x'|\alpha\rangle|^2 dx'$$

$$x|\mathbf{x}'\rangle = x'|\mathbf{x}'\rangle$$

The probability of finding the particle in all of the space

$$\int_{-\infty}^{\infty} dx'|\langle x'|\alpha\rangle|^2$$

$$y|\mathbf{x}'\rangle = y'|\mathbf{x}'\rangle$$

$$\int_{-\infty}^{\infty} dx'\langle\alpha|x'\rangle\langle x'|\alpha\rangle = 1$$

$$z|\mathbf{x}'\rangle = z'|\mathbf{x}'\rangle$$

$$\langle\alpha|\alpha\rangle = 1$$

To be able to consider such a simultaneous eigenket at all, we are implicitly assuming that the three components of the position vector can be measured simultaneously to arbitrary degrees of accuracy; hence:

$$[x_i, x_j] = 0$$

Translation

$$\mathscr{T}(d\mathbf{x}')|\mathbf{x}'\rangle = |\mathbf{x}' + d\mathbf{x}'\rangle$$

$$\mathscr{T}(d\mathbf{x}')|\alpha\rangle = \mathscr{T}(d\mathbf{x}')\int d^3x'|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle = \int d^3x'|\mathbf{x}' + d\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle$$

$$\int d^3x'|\mathbf{x}' + d\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle = \int d^3x'|\mathbf{x}'\rangle\langle\mathbf{x}' - d\mathbf{x}'|\alpha\rangle$$

$$\langle\alpha|\alpha\rangle = 1$$

1

$$\langle\alpha|\alpha\rangle = \langle\alpha|\mathscr{T}^\dagger(d\mathbf{x}')\mathscr{T}(d\mathbf{x}')|\alpha\rangle = 1 \Rightarrow \mathscr{T}^\dagger(d\mathbf{x}')\mathscr{T}(d\mathbf{x}') = 1$$

Quite generally, the norm of a ket is preserved under unitary transformations.

$$\mathscr{T}(d\mathbf{x}'')\mathscr{T}(d\mathbf{x}') = \mathscr{T}(d\mathbf{x}' + d\mathbf{x}'')$$

2

$$\mathscr{T}(-d\mathbf{x}') = \mathscr{T}^{-1}(d\mathbf{x}')$$

3

$$\lim_{d\mathbf{x}' \to 0} \mathscr{T}(d\mathbf{x}') = 1$$

4

We now demonstrate that the following infinitesimal translation operator can satisfy all the 4 mentioned properties:

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

Where, the components of K, Kx Ky, and Kz, are Hermitian operators.

1

$$\mathscr{T}^\dagger(d\mathbf{x}')\mathscr{T}(d\mathbf{x}') = (1 + i\mathbf{K}^\dagger\cdot d\mathbf{x}')(1 - i\mathbf{K}\cdot d\mathbf{x}')$$

$$= 1 - i(\mathbf{K} - \mathbf{K}^\dagger)\cdot d\mathbf{x}' + 0\left[(d\mathbf{x}')^2\right] \quad \approx 1 \quad \checkmark$$

2

$$\mathscr{T}(d\mathbf{x}'')\mathscr{T}(d\mathbf{x}') = (1 - i\mathbf{K}\cdot d\mathbf{x}'')(1 - i\mathbf{K}\cdot d\mathbf{x}')$$
$$\simeq 1 - i\mathbf{K}\cdot(d\mathbf{x}' + d\mathbf{x}'')$$
$$= \mathscr{T}(d\mathbf{x}' + d\mathbf{x}'').$$

The third and fourth properties are obvious and left for you as a practice.

What is the relation between the K and the x operators?

$$\mathbf{x}\mathscr{T}(d\mathbf{x}')|\mathbf{x}'\rangle = \mathbf{x}|\mathbf{x}'+d\mathbf{x}'\rangle = (\mathbf{x}'+d\mathbf{x}')|\mathbf{x}'+d\mathbf{x}'\rangle$$

$$\mathscr{T}(d\mathbf{x}')\mathbf{x}|\mathbf{x}'\rangle = \mathbf{x}'\mathscr{T}(d\mathbf{x}')|\mathbf{x}'\rangle = \mathbf{x}'|\mathbf{x}'+d\mathbf{x}'\rangle$$

$$[\mathbf{x},\mathscr{T}(d\mathbf{x}')]|\mathbf{x}'\rangle = d\mathbf{x}'|\mathbf{x}'+d\mathbf{x}'\rangle \simeq d\mathbf{x}'|\mathbf{x}'\rangle$$

$$[\mathbf{x},\mathscr{T}(d\mathbf{x}')] = d\mathbf{x}'$$

$$-i\mathbf{x}\mathbf{K}\cdot d\mathbf{x}' + i\mathbf{K}\cdot d\mathbf{x}'\mathbf{x} = d\mathbf{x}'$$

$$-\mathrm{i}\mathbf{x}\mathrm{K}_j\mathrm{dx}_j + \mathrm{i}\mathrm{K}_j\mathrm{dx}_j\mathbf{x} = \mathrm{dx}_j\mathbf{j}$$

$$-\mathrm{i}\mathbf{x}\mathrm{K}_j + \mathrm{i}\mathrm{K}_j\mathbf{x} = \mathbf{j}$$

$$-\mathrm{i}(\mathrm{x}_i\mathrm{K}_j - \mathrm{K}_j\mathrm{x}_i) = 0$$

$$-\mathrm{i}(\mathrm{x}_j\mathrm{K}_j - \mathrm{K}_j\mathrm{x}_j) = 1$$

$$[\mathrm{x}_i,\mathrm{K}_j] = \mathrm{i}\delta_{ij}$$

$$[\mathrm{x}_j,\mathrm{K}_j] = \mathrm{i}$$

$$[\mathrm{x}_i,\mathrm{K}_j] = 0$$