Exercise / We determine how states and operators (i.e. vectors and matrices) behave under a change of basis. In quantum mechanics, change of basis operators are unitary.

(Source: Sakurai QM, Section 1.5)

Suppose we have two orthonormal, complete sets of basis kets $\{|a\rangle\}$, $\{|b\rangle\}$:

$$\langle a^{(i)}|a^{(j)}\rangle = \delta_{ij} = \langle b^{(i)}|b^{(j)}\rangle$$

$$\mathbb{1} = \sum_i |a^{(i)}\rangle\langle a^{(i)}| = \sum_i |b^{(i)}\rangle\langle b^{(i)}|.$$

We construct a transformation operator which maps $\{|a\rangle\} \mapsto \{|b\rangle\}$.

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

Then, for all basis kets, we have

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

Furthermore, U is unitary:

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

$$\sum_k U|a^{(k)}\rangle\langle b^{(k)}| = \sum_k |b^{(k)}\rangle\langle b^{(k)}| = \mathbb{1}.$$

$$U^\dagger U = \sum_{k,l} \left(|b^{(k)}\rangle\langle a^{(k)}|\right)^\dagger \left(|b^{(l)}\rangle\langle a^{(l)}|\right) =$$

$$\sum_{k,l} |a^{(k)}\rangle\langle b^{(k)}|b^{(l)}\rangle\langle a^{(l)}| = \sum_k |a^{(k)}\rangle\langle a^{(k)}| = \mathbb{1}.$$

Therefore, we have constructed a valid change of basis operator. In the $\{|a'\rangle\}$ basis, the unitary matrix is represented as

$$U_{ij} = \langle a^{(i)}|U|a^{(j)}\rangle = \langle a^{(i)}|b^{(j)}\rangle,$$

so its entries are formed from the overlap between the old and new basis vectors.

We now determine how our change of basis operator acts on arbitrary states:

$$|\alpha\rangle = \sum_i |a^{(i)}\rangle\langle a^{(i)}|\alpha\rangle$$

The components of this state in the new basis are given by

$$\langle b^{(i)} | \alpha \rangle = \sum_j \langle b^{(i)} | a^{(j)} \rangle \langle a^{(j)} | \alpha \rangle$$

$$= U^{\dagger}_{ij} \langle a^{(j)} | \alpha \rangle \iff$$

$$\boxed{|\alpha\rangle' = U^{\dagger} |\alpha\rangle}$$

Similarly, we can express operators in the new basis as

$$\langle b^{(i)} | X | b^{(j)} \rangle = \sum_{k,l} \langle b^{(i)} | a^{(k)} \rangle \langle a^{(k)} | X | a^{(l)} \rangle \langle a^{(l)} | b^{(j)} \rangle$$

$$= \sum_{k,l} U^{\dagger}_{ik} X_{kl} U_{lj} = X'_{ij} \iff$$

$$\boxed{X' = U^{\dagger} X U.}$$

<u>TLDR</u> For two orthonormal & complete bases. $\{|a\rangle\} \xmapsto{U} \{|b\rangle\}$.

$U = \sum_k |b^{(k)}\rangle\langle a^{(k)}|$. $U_{ij} = \langle a^{(i)} | b^{(j)} \rangle$, $\langle b^{(i)} | \alpha \rangle = U^{\dagger}_{ij} \langle a^{(j)} | \alpha \rangle$

$\longleftrightarrow$ $|\alpha\rangle' = U^{\dagger} |\alpha\rangle$. $\langle b^{(i)} | X | b^{(j)} \rangle = U^{\dagger}_{ik} X_{kl} U_{lj} \longleftrightarrow X' = U^{\dagger} X U.$