Proof of Similarity Transformation relation

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Abstract

This document presents the Proof of Similarity Transformation relation.

Proof

Assume we have state vector $|\psi\rangle$ and we want to transform two orthonormal basis to each other $\{|u_i\rangle\} \rightleftharpoons \{|v_i\rangle\}$

$$|\psi\rangle_u = \sum_i c_i |u_i\rangle, \quad c_i = \langle u_i | \psi\rangle$$
 (1)

$$|\psi\rangle_v = \sum_j d_j |v_j\rangle, \quad d_j = \langle v_j | \psi\rangle$$
 (2)

Let's start with $\{|u_i\rangle\} \to \{|v_j\rangle\}$

$$d_{j} = \langle v_{j} | \psi \rangle = \langle v_{j} | \hat{\mathbf{I}} | \psi \rangle = \langle v_{j} | (\sum_{i} |u_{i}\rangle \langle u_{i}|) | \psi \rangle = \sum_{i} \langle v_{j} | u_{i}\rangle \langle u_{i} | \psi \rangle$$

According to 1 and $\langle v_j | u_i \rangle = S_{ji}$

$$d_j = \sum_i \langle v_j | u_i \rangle c_i = \sum_i S_{ji} c_i \tag{3}$$

Thus S is our Similarity Matrix, so we can say

$$|\psi\rangle_v = S \,|\psi\rangle_u \tag{4}$$

We can repeat this for $\{|v_j\rangle\} \to \{|u_i\rangle\}$

$$c_i = \langle u_i | \psi \rangle = \langle u_i | \hat{\mathbf{I}} | \psi \rangle = \langle u_i | (\sum_i |v_j\rangle \langle v_j|) | \psi \rangle = \sum_i \langle u_i | v_j \rangle \langle v_j | \psi \rangle$$

According to 2 and $\langle u_i|v_j\rangle = \langle v_j|u_i\rangle^* = S_{ji}^*$

$$c_i = \sum_j \langle u_i | v_j \rangle \, d_j = \sum_j S_{ji}^* d_j \tag{5}$$

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So we have

$$|\psi\rangle_{u} = S^{\dagger} |\psi\rangle_{u} \tag{6}$$

Now suppose we want to transform the matrix representation of an operator in one basis like \hat{A}^u to representation of that operator in another basis like \hat{A}^v

$$\hat{A}^{u} = \sum_{i,j} A^{u}_{ij} |u_{j}\rangle\langle u_{i}|, \quad A^{u}_{ij} = \langle u_{i}|\hat{A}|u_{j}\rangle$$
(7)

$$\hat{A}^{v} = \sum_{k,l} A_{kl}^{v} |v_{k}\rangle \langle v_{l}|, \quad A_{kl}^{v} = \langle v_{k}|\hat{A}|v_{l}\rangle$$
(8)

Let's start with A_{kl}^v

$$A_{kl}^{v} = \langle v_k | \hat{A} | v_l \rangle = \langle v_k | \hat{I} \hat{A} \hat{I} | v_l \rangle = \langle v_k | \left(\sum_i |u_i\rangle \langle u_i| \right) \hat{A} \left(\sum_j |u_j\rangle \langle u_j| \right) |v_l\rangle$$
$$= \sum_i \langle v_k |u_i\rangle \langle u_i | \hat{A} |u_j\rangle \langle u_j |v_l\rangle$$

According to 7, $\langle v_k | u_i \rangle = S_{ki}$ and $\langle u_j | v_l \rangle = S_{lj}^*$, we can write

$$A_{kl}^{v} = \sum_{i,j} \langle v_k | u_i \rangle \langle u_i | A | u_j \rangle \langle u_j | v_l \rangle = \sum_{i,j} S_{ki} A_{ij}^{u} S_{lj}^{*}$$

$$(9)$$

Thus S is our Similarity Matrix, so we can say

$$\hat{A}^v = S\hat{A}^u S^\dagger \tag{10}$$

We can repeat this for A_{ij}^u

$$\begin{aligned} \mathbf{A}_{ij}^{u} &= \langle u_{i} | \hat{\mathbf{A}} | u_{j} \rangle = \langle u_{i} | \hat{\mathbf{I}} \hat{\mathbf{A}} \hat{\mathbf{I}} | u_{j} \rangle = \langle u_{i} | \left(\sum_{k} |v_{k}\rangle\langle v_{k}| \right) \hat{\mathbf{A}} \left(\sum_{l} |v_{l}\rangle\langle v_{l}| \right) | u_{j} \rangle \\ &= \sum_{k,l} \langle u_{i} | v_{k} \rangle \langle v_{k} | \hat{\mathbf{A}} | v_{l} \rangle \langle v_{l} | u_{j} \rangle \end{aligned}$$

According to 8, $\langle u_i | v_k \rangle = S_{ki}^*$ and $\langle u_l | v_j \rangle = S_{lj}$, we can write

$$A_{ij}^{u} = \sum_{k,l} \langle u_i | v_k \rangle \langle v_k | \hat{A} | v_l \rangle \langle v_l | u_j \rangle = \sum_{k,l} S_{ki}^* A_{kl}^v S_{lj}$$
(11)

Thus S is our Similarity Matrix, so we can say

$$\hat{A}^u = S^{\dagger} \hat{A}^v S \tag{12}$$