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General notes from research
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1 Nonorthogonal bases

Reference:
https://www.tcm.phy.cam.ac.uk/∼pdh1001/thesis/node26.html

A lot of the expressions we're used to seeing in orthogonal bases change a little when using nonorthogonal bases. It's useful to define the overlap matrix:

$$S_{ij} = \langle \phi_i | \phi_j \rangle$$

In the case of an orthogonal matrix it is the identity, and later on, we'll see it can play the role of a metric.

1.1 Resolution of the identity

The resolution of the identity changes with an overlap matrix. The normal resolution of the identity is

$$\sum_i |\phi_i\rangle\langle\phi_i| = \mathbf{1}$$

This works because this operator that we defined acts the same as the identity operator on an arbitrary vector, $|v\rangle$:

$$|v\rangle = \sum_i |\phi_i\rangle\langle\phi_i|v\rangle$$

This is true because it is simply the result of expanding the vector in that basis:

$$\begin{aligned} |v\rangle &\equiv \sum_j |\phi_j\rangle c_j \\ \langle\phi_i|v\rangle &= \sum_j \langle\phi_i|\phi_j\rangle c_j = \sum_j \delta_{ij} c_j = c_i \end{aligned}$$

Note the appearance of δ_{ij} is directly from orthogonality.

To generalize this expression, imagine trying to perform the same steps:

$$\begin{aligned} |v\rangle &\equiv \sum_j |\varphi_j\rangle c_j \\ \langle\varphi_i|v\rangle &= \sum_j \langle\varphi_i|\varphi_j\rangle c_j = \sum_j S_{ij} c_j = Sc \\ \implies \sum_i S^{-1}_{ki}\langle\varphi_i|v\rangle &= \sum_{ij} S^{-1}_{ki} S_{ij} c_j = \sum_j \delta_{kj} c_j = c_k \\ \implies |v\rangle &= \sum_{ij} |\varphi_j\rangle S^{-1}_{ji}\langle\varphi_i|v\rangle \\ \implies \sum_{ij} |\varphi_i\rangle S^{-1}_{ij}\langle\varphi_j| &= \mathbf{1} \end{aligned}$$

The final statement is the new resolution of the identity.

1.2 Change of basis matrix

Now that I have the resolution of the identity, changing bases is easy. In the case of orthogonal basis:

$$|v\rangle = \sum_i |\phi_i\rangle\langle\phi_i|v\rangle \equiv |\phi_i\rangle v_i^\phi$$

This is the representation of $|v\rangle$ in the $|\phi_i\rangle$ basis. The column vector is the list $(\langle\phi_1|v\rangle, ..., \langle\phi_N|v\rangle)$. With another orthogonal basis, $|\theta_i\rangle$,

$$|v\rangle = \sum_{ij} |\theta_i\rangle\langle\theta_i|\phi_j\rangle\langle\phi_j|v\rangle = \sum_{ij} |\theta_i\rangle A_{ij} v_j^\phi \equiv \sum_i |\theta_i\rangle v_i^\theta$$

where A_{ij} is the change-of-basis from ϕ-basis to θ-basis, and

$$A_{ij} \equiv \langle\theta_i|\phi_j\rangle$$

Notice the columns of this matrix are the representations of $|\phi_j\rangle$ in the θ-basis. If the vector space is real, then the rows are representations of $|\theta_i\rangle$ in the ϕ-basis.

In the case of a nonorthogonal basis, $|\varphi_i\rangle$, the identity is different. The expression for the vector is

$$|v\rangle = \sum_{ij} |\varphi_i\rangle S_{ij}^{-1}\langle\varphi_j|v\rangle \equiv \sum_i |\varphi_i\rangle v_i^\varphi$$

So now the components are $v_i^\varphi \equiv S_{ij}^{-1}\langle\varphi_j|v\rangle$. Another nonorthogonal basis will have another overlap matrix: $Q_{ij} \equiv \langle\vartheta_i|\vartheta_j\rangle$.

$$|v\rangle = \sum_{kli} |\vartheta_k\rangle Q_{kl}^{-1}\langle\vartheta_l|\varphi_i\rangle v_i^\varphi \equiv \sum_k |\vartheta_k\rangle B_{ki} v_i^\varphi \equiv \sum_k |\vartheta_k\rangle v_k^\vartheta$$

Now

$$B_{ki} \equiv Q_{kl}^{-1}\langle\vartheta_l|\varphi_i\rangle$$

is the change-of-basis matrix from the φ-basis to the ϑ-basis. Note that, like before, the columns of B are the representations of $|\varphi_i\rangle$ in the ϑ-basis.

For a more concrete example, working only with numbers and no abstract vectors, consider if you have a vector represented in an nonorthogonal basis set. I'm going to use Einstein notation for the rest of the section. This means you have the numbers $v_i^\varphi = \sum_j S_{ij}^{-1}\langle\varphi_j|v\rangle$. Now you want the representation in an orthogonal basis set, $v_i^\phi = \langle\phi_i|v\rangle$, and you know the orthogonal basis elements represented in the nonorthogonal basis set: $[\phi_k^\varphi]_i = S_{ij}^{-1}\langle\varphi_j|\phi_k\rangle$. The relationship between the two can be drawn as follows:

$$\begin{aligned}\langle\phi_i|v\rangle &= \langle\phi_i|\varphi_j\rangle S_{jk}^{-1}\langle\varphi_k|v\rangle = \langle\phi_i|\varphi_j\rangle S_{jk}^{-1}\delta_{kl}\langle\varphi_l|v\rangle = \langle\phi_i|\varphi_j\rangle S_{jk}^{-1} S_{km} S_{ml}^{-1}\langle\varphi_l|v\rangle \\ &= [\phi_i^\varphi]_k S_{km} v_m^\varphi\end{aligned}$$

The extra S comes about by needing to provide an S^{-1} for our two representations of vectors in the nonorthogonal basis.