D matrix calculations

We want to show that the following equation:

$$U = U_0 + \frac{1}{2} \sum_{\bar{R}\bar{R}'} \sum_{\alpha\beta} u_\alpha(\bar{R}) D_{\alpha\beta}(\bar{R}-\bar{R}') u_\beta(\bar{R}')$$

Where:

$$D_{\alpha\beta}(\bar{R}-\bar{R}') = \delta_{\bar{R}\bar{R}'} \left[\sum_{\bar{R}''} \Phi_{\alpha\beta}(\bar{R}-\bar{R}'')\right] - \Phi_{\alpha\beta}(\bar{R}-\bar{R}')$$

Is equivalent to:

$$U = U_0 + \frac{1}{4} \sum_{\bar{R}\bar{R}'} \sum_{\alpha\beta} (u_\alpha(\bar{R}) - u_\alpha(\bar{R}')) \Phi_{\alpha\beta}(\bar{R}-\bar{R}')(u_\beta(\bar{R}) - u_\beta(\bar{R}'))$$

Let's go. But first we make a slight notation change to simplify the writing:

$$u_\alpha(\bar{R}) \equiv u_\alpha \qquad u_\alpha(\bar{R}') \equiv u'_\alpha$$

By substitution we obtain:

$$U = U_0 + \frac{1}{2} \sum_{\bar{R}\bar{R}'} \sum_{\alpha\beta} u_\alpha \left[\delta_{\bar{R}\bar{R}'} \left[\sum_{\bar{R}''} \Phi_{\alpha\beta}(\bar{R}-\bar{R}'')\right] - \Phi_{\alpha\beta}(\bar{R}-\bar{R}')\right] u'_\beta$$

$$U = U_0 + \frac{1}{2} \sum_{\alpha\beta} \left[\sum_{\bar{R}\bar{R}'\bar{R}''} u_\alpha \delta_{\bar{R}\bar{R}'} \Phi_{\alpha\beta}(\bar{R}-\bar{R}'') u'_\beta - \sum_{\bar{R}\bar{R}'} u_\alpha \Phi_{\alpha\beta}(\bar{R}-\bar{R}') u'_\beta\right]$$

I can now sum either over R or over R'.
I begin by summing over R':

$$U = U_0 + \frac{1}{2} \sum_{\alpha\beta} \left[\sum_{\bar{R}\bar{R}''} u_\alpha \Phi_{\alpha\beta}(\bar{R}-\bar{R}'') u_\beta - \sum_{\bar{R}\bar{R}'} u_\alpha \Phi_{\alpha\beta}(\bar{R}-\bar{R}') u'_\beta\right]$$

Relabel
$\bar{R}'' \to \bar{R}'$

$$U = U_0 + \frac{1}{2} \sum_{\alpha\beta} \left[\sum_{\bar{R}\bar{R}'} u_\alpha \Phi_{\alpha\beta}(\bar{R}-\bar{R}') u_\beta - \sum_{\bar{R}\bar{R}'} u_\alpha \Phi_{\alpha\beta}(\bar{R}-\bar{R}') u'_\beta\right]$$

$$U = U_0 + \frac{1}{2} \sum_{\alpha\beta} \sum_{\bar{R}\bar{R}'} u_\alpha \Phi_{\alpha\beta}(\bar{R}-\bar{R}') (u_\beta - u'_\beta) \qquad \mathrm{I}$$

If I instead sum over R

$$U = U_0 + \frac{1}{2} \sum_{\alpha\beta} \left[\sum_{\bar{R}'\bar{R}''} u'_\alpha \Phi_{\alpha\beta}(\bar{R}'-\bar{R}'') u'_\beta - \sum_{\bar{R}\bar{R}'} u_\alpha \Phi_{\alpha\beta}(\bar{R}-\bar{R}') u'_\beta\right]$$

Relabeling
$\bar{R}'' \to \bar{R}$

$$U = U_0 + \frac{1}{2} \sum_{\alpha\beta} \left[\sum_{\bar{R}'\bar{R}} u'_\alpha \Phi_{\alpha\beta}(\bar{R}'-\bar{R}) u'_\beta - \sum_{\bar{R}\bar{R}'} u_\alpha \Phi_{\alpha\beta}(\bar{R}-\bar{R}') u'_\beta\right]$$

Now we use the inversion property:

$$\Phi_{\alpha\beta}(\bar{R}-\bar{R}') = \Phi_{\alpha\beta}(\bar{R}'-\bar{R})$$

To obtain the expression:

$$U = U_0 + \frac{1}{2}\sum_{\alpha\beta}\left[\sum_{\bar{R}'\bar{R}} u'_\alpha \, \Phi_{\alpha\beta}(\bar{R}'-\bar{R})\, u'_\beta - \sum_{\bar{R}\bar{R}'} u_\alpha \, \Phi_{\alpha\beta}(\bar{R}'-\bar{R})\, u'_\beta\right]$$

$$U = U_0 + \frac{1}{2}\sum_{\alpha\beta}\left[\sum_{\bar{R}'\bar{R}} (u'_\alpha - u_\alpha)\, \Phi_{\alpha\beta}(\bar{R}'-\bar{R})\, u'_\beta\right]$$

$$U = U_0 - \frac{1}{2}\sum_{\alpha\beta}\left[\sum_{\bar{R}'\bar{R}} (u_\alpha - u'_\alpha)\, \Phi_{\alpha\beta}(\bar{R}'-\bar{R})\, u'_\beta\right]$$

Now we use symmetry+inversion

$$\Phi_{\alpha\beta}(\bar{R}-\bar{R}') = \Phi_{\beta\alpha}(\bar{R}'-\bar{R})$$

We have then:

$$U = U_0 - \frac{1}{2}\sum_{\alpha\beta}\left[\sum_{\bar{R}'\bar{R}} (u_\alpha - u'_\alpha)\, \Phi_{\beta\alpha}(\bar{R}-\bar{R}')\, u'_\beta\right]$$ Reordering

$$U = U_0 - \frac{1}{2}\sum_{\alpha\beta}\left[\sum_{\bar{R}'\bar{R}} u'_\beta\, \Phi_{\beta\alpha}(\bar{R}-\bar{R}')(u_\alpha - u'_\alpha)\right]$$ Relabeling $\alpha \to \mu$, $\beta \to \nu$ Just for ease

$$U = U_0 - \frac{1}{2}\sum_{\mu\nu}\left[\sum_{\bar{R}'\bar{R}} u'_\mu\, \Phi_{\mu\nu}(\bar{R}-\bar{R}')(u_\nu - u'_\nu)\right]$$ II

Finally we can add equation I and II to obtain

$$2U = 2U_0 + \frac{1}{2}\sum_{\alpha\beta}\sum_{\bar{R}\bar{R}'} (u_\alpha - u'_\alpha)\, \Phi_{\alpha\beta}(\bar{R}-\bar{R}')\,(u_\beta - u'_\beta)$$

$$U = U_0 + \frac{1}{4}\sum_{\alpha\beta}\sum_{\bar{R}\bar{R}'} (u_\alpha - u'_\alpha)\, \Phi_{\alpha\beta}(\bar{R}-\bar{R}')\,(u_\beta - u'_\beta)$$