# Derivation of the equation of motion for a 3d harmonic crystal

We want to show that a 3d harmonic crystal obeys the following equation of motion:

$$M\ddot{\bar{u}}(\bar{R}) = -\sum_{\bar{R}'} D(\bar{R}-\bar{R}')\bar{u}(\bar{R}')$$

Or equivalently

$$M\ddot{u}_\alpha(\bar{R}) = -\sum_{\bar{R}'}\sum_{\beta} D_{\alpha\beta}(\bar{R}-\bar{R}')u_\beta(\bar{R}')$$

We proceed by using the nuclear motion in the Born-Oppenheimer framework:

$$M\ddot{u}_\gamma(\bar{R}'') = -\frac{\partial U}{\partial u_\gamma(\bar{R}'')}$$

Where

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

So we obtain

$$M\ddot{u}_\gamma(\bar{R}'') = -\frac{\partial}{\partial u_\gamma(\bar{R}'')}\left[U_0 + \frac{1}{2}\sum_{\bar{R}\bar{R}'}\sum_{\alpha\beta} u_\alpha D_{\alpha\beta}(\bar{R}-\bar{R}')u'_\beta\right] \qquad \frac{\partial u_\alpha(\bar{R})}{\partial u_\beta(\bar{R}')} = \delta_{\alpha\beta}\delta_{\bar{R}\bar{R}'}$$

$$M\ddot{u}_\gamma(\bar{R}'') = -\frac{1}{2}\sum_{\bar{R}\bar{R}'}\sum_{\alpha\beta}\left[\delta_{\alpha\gamma}\delta_{\bar{R}\bar{R}''}D_{\alpha\beta}(\bar{R}-\bar{R}')u'_\beta + u_\alpha D_{\alpha\beta}(\bar{R}-\bar{R}')\delta_{\beta\gamma}\delta_{\bar{R}'\bar{R}''}\right]$$

$$M\ddot{u}_\gamma(\bar{R}'') = -\frac{1}{2}\left[\sum_{\bar{R}'}\sum_{\beta} D_{\gamma\beta}(\bar{R}''-\bar{R}')u'_\beta + \sum_{\bar{R}}\sum_{\alpha} u_\alpha D_{\alpha\gamma}(\bar{R}-\bar{R}'')\right] \qquad \text{Relabeling } \bar{R}'\to\bar{R}$$

$$M\ddot{u}_\gamma(\bar{R}'') = -\frac{1}{2}\left[\sum_{\bar{R}}\sum_{\beta} D_{\gamma\beta}(\bar{R}''-\bar{R})u_\beta + \sum_{\bar{R}}\sum_{\alpha} u_\alpha D_{\alpha\gamma}(\bar{R}-\bar{R}'')\right]$$

$$M\ddot{u}_\gamma(\bar{R}'') = -\frac{1}{2}\left[\sum_{\bar{R}}\sum_{\beta} D_{\gamma\beta}(\bar{R}''-\bar{R})u_\beta + \sum_{\bar{R}}\sum_{\alpha} D_{\alpha\gamma}(\bar{R}-\bar{R}'')u_\alpha\right]$$

Now we use the the simmetry property of the D matrix

$$D_{\alpha\gamma}(\bar{R}-\bar{R}'') = D_{\gamma\alpha}(\bar{R}''-\bar{R})$$

To obtain

$$M\ddot{u}_\gamma(\bar{R}'') = -\frac{1}{2}\left[\sum_{\bar{R}}\sum_{\beta} D_{\gamma\beta}(\bar{R}''-\bar{R})u_\beta + \sum_{\bar{R}}\sum_{\alpha} D_{\gamma\alpha}(\bar{R}''-\bar{R})u_\alpha\right]$$

Now we can interchange the index without problems

$$M \ddot{u}_\gamma(\bar{R}'') = -\sum_{\bar{R}} \sum_{\beta} D_{\gamma\beta}(\bar{R}'' - \bar{R})\, u_\beta$$