Phonon dispersion relation of a bcc lattice:

Equation of motion in x -direction is:

$$
\begin{aligned}
&\frac{d^2u^x_{lmn}}{dt^2} = \frac{C}{\sqrt{3}\ m}[(u^x_{l+1m+1n+1} - u^x_{lmn}) + (u^x_{l-1m+1n+1} - u^x_{lmn}) + (u^x_{l-1m-1n+1} - u^x_{lmn})+\\
&+(u^x_{l+1m-1n+1} - u^x_{lmn}) + (u^x_{l+1m+1n-1} - u^x_{lmn}) + (u^x_{l-1m+1n-1} - u^x_{lmn}) + (u^x_{l-1m-1n-1} - u^x_{lmn})+\\
&+(u^x_{l+1m-1n-1} - u^x_{lmn}) + (u^y_{l+1m+1n+1} - u^y_{lmn}) - (u^y_{l-1m+1n+1} - u^y_{lmn}) - (u^y_{l-1m-1n+1} - u^y_{lmn})+\\
&+(u^y_{l+1m-1n+1} - u^y_{lmn}) - (u^y_{l+1m+1n-1} - u^y_{lmn}) + (u^y_{l-1m+1n-1} - u^y_{lmn}) - (u^y_{l-1m-1n-1} - u^y_{lmn})+\\
&+(u^y_{l+1m-1n-1} - u^y_{lmn}) + (u^z_{l+1m+1n+1} - u^z_{lmn}) - (u^z_{l-1m+1n+1} - u^z_{lmn}) - (u^z_{l-1m-1n+1} - u^z_{lmn})+\\
&+(u^z_{l+1m-1n+1} - u^z_{lmn}) - (u^z_{l+1m+1n-1} - u^z_{lmn}) + (u^z_{l-1m+1n-1} - u^z_{lmn}) + (u^z_{l-1m-1n-1} - u^z_{lmn})-\\
&-(u^z_{l+1m-1n-1} - u^z_{lmn})]
\end{aligned}
$$

For u^x_{lmn}

$$u^x_{lmn} = u^x_{\overrightarrow{k}} e^{i(\sum_{i=1}^{3}\ \overrightarrow{a_i}\overrightarrow{k}\ -\ \omega t)}$$

was used.

Primitve vectors for bcc are:

$$A = \frac{a}{2}\begin{bmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix}$$

We obtain:

$$u^x_{lmn} = u^x_{\overrightarrow{k}} e^{i(l\overrightarrow{k}\cdot\overrightarrow{a_1} + m\overrightarrow{k}\cdot\overrightarrow{a_2} + n\overrightarrow{k}\cdot\overrightarrow{a_3})} = u^x_{\overrightarrow{k}} e^{i(\frac{(-l+m+n)k_x a}{2} + \frac{(l-m+n)k_y a}{2} + \frac{(l+m-n)k_z a}{2})}$$

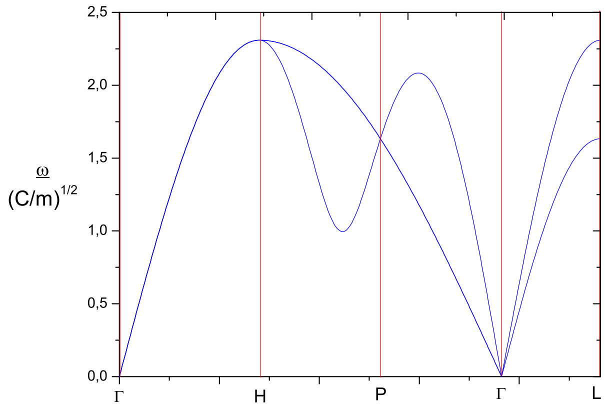

Figure 1: Phonon dispersion of a bcc lattice. Plot is over the symmetry lines as follows: gamma - H - P - gamma - N

On the next page solutions of the equation of motion are summed up in a array.

$$
\begin{bmatrix}
\begin{array}{l} 4 - cos(\frac{a}{2}(k_x + k_y + k_z)) - cos(\frac{a}{2}(3k_x - k_y - k_z)) \\ -cos(\frac{a}{2}(-k_x + 3k_y - k_z)) - cos(\frac{a}{2}(-k_x - k_y + 3k_z)) - \frac{m\omega^2}{\sqrt{3}C} \end{array} &
\begin{array}{l} -cos(\frac{a}{2}(k_x + k_y + k_z)) + cos(\frac{a}{2}(3k_x - k_y - k_z)) \\ +cos(\frac{a}{2}(-k_x + 3k_y - k_z)) - cos(\frac{a}{2}(-k_x - k_y + 3k_z)) \end{array} &
\begin{array}{l} -cos(\frac{a}{2}(k_x + k_y + k_z)) + cos(\frac{a}{2}(3k_x - k_y - k_z)) \\ -cos(\frac{a}{2}(-k_x + 3k_y - k_z)) + cos(\frac{a}{2}(-k_x - k_y + 3k_z)) \end{array} \\
\begin{array}{l} -cos(\frac{a}{2}(k_x + k_y + k_z)) + cos(\frac{a}{2}(3k_x - k_y - k_z)) \\ +cos(\frac{a}{2}(-k_x + 3k_y - k_z)) - cos(\frac{a}{2}(-k_x - k_y + 3k_z)) \end{array} &
\begin{array}{l} 4 - cos(\frac{a}{2}(k_x + k_y + k_z)) - cos(\frac{a}{2}(3k_x - k_y - k_z)) \\ -cos(\frac{a}{2}(-k_x + 3k_y - k_z)) - cos(\frac{a}{2}(-k_x - k_y + 3k_z)) - \frac{m\omega^2}{\sqrt{3}C} \end{array} &
\begin{array}{l} -cos(\frac{a}{2}(k_x + k_y + k_z)) - cos(\frac{a}{2}(3k_x - k_y - k_z)) \\ +cos(\frac{a}{2}(-k_x + 3k_y - k_z)) + cos(\frac{a}{2}(-k_x - k_y + 3k_z)) \end{array} \\
\begin{array}{l} -cos(\frac{a}{2}(k_x + k_y + k_z)) + cos(\frac{a}{2}(3k_x - k_y - k_z)) \\ -cos(\frac{a}{2}(-k_x + 3k_y - k_z)) + cos(\frac{a}{2}(-k_x - k_y + 3k_z)) \end{array} &
\begin{array}{l} -cos(\frac{a}{2}(k_x + k_y + k_z)) - cos(\frac{a}{2}(3k_x - k_y - k_z)) \\ +cos(\frac{a}{2}(-k_x + 3k_y - k_z)) + cos(\frac{a}{2}(-k_x - k_y + 3k_z)) \end{array} &
\begin{array}{l} 4 - cos(\frac{a}{2}(k_x + k_y + k_z)) - cos(\frac{a}{2}(3k_x - k_y - k_z)) \\ -cos(\frac{a}{2}(-k_x + 3k_y - k_z)) - cos(\frac{a}{2}(-k_x - k_y + 3k_z)) - \frac{m\omega^2}{\sqrt{3}C} \end{array}
\end{bmatrix} =
$$

$$0$$