

We seek the phonon dispersion curves for a crystal of Cu (which forms an fcc lattice) in the  $[110]$  direction in  $k$ -space. A general vector that points in that direction is given by:

$$\mathbf{k} = \frac{k}{\sqrt{2}}(\hat{i} + \hat{j}) \quad (1)$$

The expression for the force on the atom located at the origin due to it's motion and the motion of on of it's neighbors is given by:

$$\mathbf{F} = -\alpha \left[ \hat{\mathbf{R}} \cdot \mathbf{u}(000) - \hat{\mathbf{R}} \cdot \mathbf{u}(\mathbf{R}) \right] \hat{\mathbf{R}} \quad (2)$$

Each cu atom has 12 nearest neighbors. They are located at:

$$a\left(\frac{1}{2}\frac{1}{2}0\right) \quad a\left(\frac{1}{2}0\frac{1}{2}\right) \quad a\left(0\frac{1}{2}\frac{1}{2}\right) \quad (3)$$

$$a\left(-\frac{1}{2}\frac{1}{2}0\right) \quad a\left(-\frac{1}{2}0\frac{1}{2}\right) \quad a\left(0-\frac{1}{2}\frac{1}{2}\right) \quad (4)$$

$$a\left(\frac{1}{2}-\frac{1}{2}0\right) \quad a\left(\frac{1}{2}0-\frac{1}{2}\right) \quad a\left(0\frac{1}{2}-\frac{1}{2}\right) \quad (5)$$

$$a\left(-\frac{1}{2}-\frac{1}{2}0\right) \quad a\left(-\frac{1}{2}0-\frac{1}{2}\right) \quad a\left(0-\frac{1}{2}-\frac{1}{2}\right) \quad (6)$$

$$(7)$$

Let's attack them one at a time.

For  $\mathbf{r}_n = a\left(\frac{1}{2}\frac{1}{2}0\right)$ :

$$\hat{\mathbf{R}} = \frac{1}{\sqrt{2}}(\hat{i} + \hat{j}) \quad (8)$$

and assuming

$$\mathbf{u}_n = \mathbf{A}e^{i\mathbf{k} \cdot \mathbf{r}_n - i\omega t} \quad (9)$$

$$= \mathbf{A}e^{i\left(\frac{ka}{2\sqrt{2}} + \frac{ka}{2\sqrt{2}}\right) - i\omega t} \quad (10)$$

$$= \mathbf{A}e^{i\left(\frac{ka}{\sqrt{2}}\right) - i\omega t} \quad (11)$$

$$= \mathbf{u}(000)e^{i\left(\frac{ka}{\sqrt{2}}\right)} \quad (12)$$

$$(13)$$

$$\mathbf{F} = -\alpha \left[ \hat{\mathbf{R}} \cdot \mathbf{u}(000) - \hat{\mathbf{R}} \cdot \mathbf{u}(\mathbf{R}) \right] \hat{\mathbf{R}} \quad (14)$$

$$= -\alpha \left[ \frac{1}{\sqrt{2}}(\hat{i} + \hat{j}) \cdot \mathbf{u}(000) - \frac{1}{\sqrt{2}}(\hat{i} + \hat{j}) \cdot \mathbf{u}\left(\frac{1}{2} \frac{1}{2} 0\right) \right] \frac{1}{\sqrt{2}}(\hat{i} + \hat{j}) \quad (15)$$

$$= -\frac{\alpha}{2} \left[ (\hat{i} + \hat{j}) \cdot \mathbf{u}(000) - (\hat{i} + \hat{j}) \cdot \mathbf{u}\left(\frac{1}{2} \frac{1}{2} 0\right) \right] (\hat{i} + \hat{j}) \quad (16)$$

$$= -\frac{\alpha}{2} \left[ u_x(000) + u_y(000) - u_x(000)e^{i(\frac{ka}{\sqrt{2}})} - u_y(000)e^{i(\frac{ka}{\sqrt{2}})} \right] (\hat{i} + \hat{j}) \quad (17)$$

$$= -\frac{\alpha}{2} \left[ u_x(000) \left(1 - e^{i(\frac{ka}{\sqrt{2}})}\right) + u_y(000) \left(1 - e^{i(\frac{ka}{\sqrt{2}})}\right) \right] (\hat{i} + \hat{j}) \quad (18)$$

$$(19)$$

For  $\mathbf{r}_n = a(-\frac{1}{2} \frac{1}{2} 0)$ :

$$\hat{\mathbf{R}} = \frac{1}{\sqrt{2}}(-\hat{i} + \hat{j}) \quad (20)$$

and assuming

$$\mathbf{u}\left(-\frac{1}{2} \frac{1}{2} 0\right) = \mathbf{A}e^{i\mathbf{k} \cdot \mathbf{r}_n - i\omega t} \quad (21)$$

$$= \mathbf{A}e^{i\left(\frac{-ka}{2\sqrt{2}} + \frac{ka}{2\sqrt{2}}\right) - i\omega t} \quad (22)$$

$$= \mathbf{A}e^{i0 - i\omega t} \quad (23)$$

$$= \mathbf{u}(000) \quad (24)$$

$$(25)$$

$$\mathbf{F} = -\alpha \left[ \hat{\mathbf{R}} \cdot \mathbf{u}(000) - \hat{\mathbf{R}} \cdot \mathbf{u}(\mathbf{R}) \right] \hat{\mathbf{R}} \quad (26)$$

$$= -\alpha \left[ \frac{1}{\sqrt{2}}(-\hat{i} + \hat{j}) \cdot \mathbf{u}(000) - \frac{1}{\sqrt{2}}(-\hat{i} + \hat{j}) \cdot \mathbf{u}\left(-\frac{1}{2} \frac{1}{2} 0\right) \right] \frac{1}{\sqrt{2}}(-\hat{i} + \hat{j}) \quad (27)$$

$$= -\frac{\alpha}{2} \left[ (-\hat{i} + \hat{j}) \cdot \mathbf{u}(000) - (-\hat{i} + \hat{j}) \cdot \mathbf{u}\left(-\frac{1}{2} \frac{1}{2} 0\right) \right] (-\hat{i} + \hat{j}) \quad (28)$$

$$= -\frac{\alpha}{2} [-u_x(000) + u_y(000) + u_x(000) - u_y(000)] (-\hat{i} + \hat{j}) \quad (29)$$

$$= 0 \quad (30)$$

For  $\mathbf{r}_n = a(\frac{1}{2} - \frac{1}{2} 0)$ :

$$\hat{\mathbf{R}} = \frac{1}{\sqrt{2}}(\hat{i} - \hat{j}) \quad (31)$$

and assuming

$$\mathbf{u}\left(\frac{1}{2}, -\frac{1}{2}, 0\right) = \mathbf{A}e^{i\mathbf{k}\cdot\mathbf{r}_n - i\omega t} \quad (32)$$

$$= \mathbf{A}e^{i\left(\frac{ka}{2\sqrt{2}} - \frac{ka}{2\sqrt{2}}\right) - i\omega t} \quad (33)$$

$$= \mathbf{A}e^{i0 - i\omega t} \quad (34)$$

$$= \mathbf{u}(000) \quad (35)$$

$$(36)$$

$$\mathbf{F} = -\alpha \left[ \hat{\mathbf{R}} \cdot \mathbf{u}(000) - \hat{\mathbf{R}} \cdot \mathbf{u}(\mathbf{R}) \right] \hat{\mathbf{R}} \quad (37)$$

$$= -\alpha \left[ \frac{1}{\sqrt{2}}(\hat{i} - \hat{j}) \cdot \mathbf{u}(000) - \frac{1}{\sqrt{2}}(\hat{i} - \hat{j}) \cdot \mathbf{u}\left(\frac{1}{2}, -\frac{1}{2}, 0\right) \right] \frac{1}{\sqrt{2}}(\hat{i} - \hat{j}) \quad (38)$$

$$= -\frac{\alpha}{2} \left[ (\hat{i} - \hat{j}) \cdot \mathbf{u}(000) - (\hat{i} - \hat{j}) \cdot \mathbf{u}\left(\frac{1}{2}, -\frac{1}{2}, 0\right) \right] (\hat{i} - \hat{j}) \quad (39)$$

$$= -\frac{\alpha}{2} [u_x(000) - u_y(000) - u_x(000) + u_y(000)] (\hat{i} - \hat{j}) \quad (40)$$

$$= 0 \quad (41)$$

$$(42)$$

Makes sense since these atoms lie on the same wavefront and so should always be in phase with the atom at the origin.

For  $\mathbf{r}_n = a(-\frac{1}{2}, -\frac{1}{2}, 0)$ :

$$\hat{\mathbf{R}} = \frac{1}{\sqrt{2}}(-\hat{i} - \hat{j}) \quad (43)$$

and assuming

$$\mathbf{u}\left(-\frac{1}{2}, -\frac{1}{2}, 0\right) = \mathbf{A}e^{i\mathbf{k}\cdot\mathbf{r}_n - i\omega t} \quad (44)$$

$$= \mathbf{A}e^{i\left(\frac{-ka}{2\sqrt{2}} - \frac{ka}{2\sqrt{2}}\right) - i\omega t} \quad (45)$$

$$= \mathbf{A}e^{i\frac{-ka}{\sqrt{2}} - i\omega t} \quad (46)$$

$$= \mathbf{u}(000)e^{i\frac{-ka}{\sqrt{2}}} \quad (47)$$

$$(48)$$

$$\mathbf{F} = -\alpha \left[ \hat{\mathbf{R}} \cdot \mathbf{u}(000) - \hat{\mathbf{R}} \cdot \mathbf{u}(\mathbf{R}) \right] \hat{\mathbf{R}} \quad (49)$$

$$= -\alpha \left[ \frac{1}{\sqrt{2}}(-\hat{i} - \hat{j}) \cdot \mathbf{u}(000) - \frac{1}{\sqrt{2}}(-\hat{i} - \hat{j}) \cdot \mathbf{u}\left(-\frac{1}{2}, -\frac{1}{2}, 0\right) \right] \frac{1}{\sqrt{2}}(-\hat{i} - \hat{j}) \quad (50)$$

$$= -\frac{\alpha}{2} \left[ (-\hat{i} - \hat{j}) \cdot \mathbf{u}(000) - (-\hat{i} - \hat{j}) \cdot \mathbf{u}\left(-\frac{1}{2}, -\frac{1}{2}, 0\right) \right] (-\hat{i} - \hat{j}) \quad (51)$$

$$= -\frac{\alpha}{2} \left[ -u_x(000) - u_y(000) + u_x(000)e^{-i\frac{ka}{\sqrt{2}}} + u_y(000)e^{-i\frac{ka}{\sqrt{2}}} \right] (-\hat{i} - \hat{j}) \quad (52)$$

$$= -\frac{\alpha}{2} \left[ u_x(000) \left( -1 + e^{-i(\frac{ka}{\sqrt{2}})} \right) + u_y(000) \left( -1 + e^{-i(\frac{ka}{\sqrt{2}})} \right) \right] (-\hat{i} - \hat{j}) \quad (53)$$

$$(54)$$

For  $\mathbf{r}_n = a(\frac{1}{2}, 0, \frac{1}{2})$ :

$$\hat{\mathbf{R}} = \frac{1}{\sqrt{2}}(\hat{i} + \hat{k}) \quad (55)$$

and assuming

$$\mathbf{u}\left(\frac{1}{2}, 0, \frac{1}{2}\right) = \mathbf{A}e^{i\mathbf{k} \cdot \mathbf{r}_n - i\omega t} \quad (56)$$

$$= \mathbf{A}e^{i(\frac{ka}{2\sqrt{2}} + 0) - i\omega t} \quad (57)$$

$$= \mathbf{A}e^{i\frac{ka}{2\sqrt{2}} - i\omega t} \quad (58)$$

$$= \mathbf{u}(000)e^{i\frac{ka}{2\sqrt{2}}} \quad (59)$$

$$(60)$$

$$\mathbf{F} = -\alpha \left[ \hat{\mathbf{R}} \cdot \mathbf{u}(000) - \hat{\mathbf{R}} \cdot \mathbf{u}(\mathbf{R}) \right] \hat{\mathbf{R}} \quad (61)$$

$$= -\alpha \left[ \frac{1}{\sqrt{2}}(\hat{i} + \hat{k}) \cdot \mathbf{u}(000) - \frac{1}{\sqrt{2}}(\hat{i} + \hat{k}) \cdot \mathbf{u}\left(\frac{1}{2}, 0, \frac{1}{2}\right) \right] \frac{1}{\sqrt{2}}(\hat{i} + \hat{k}) \quad (62)$$

$$= -\frac{\alpha}{2} \left[ (\hat{i} + \hat{k}) \cdot \mathbf{u}(000) - (\hat{i} + \hat{k}) \cdot \mathbf{u}\left(\frac{1}{2}, 0, \frac{1}{2}\right) \right] (\hat{i} + \hat{k}) \quad (63)$$

$$= -\frac{\alpha}{2} \left[ u_x(000) + u_z(000) - u_x(000)e^{i\frac{ka}{2\sqrt{2}}} - u_z(000)e^{i\frac{ka}{2\sqrt{2}}} \right] (\hat{i} + \hat{k}) \quad (64)$$

$$= -\frac{\alpha}{2} \left[ u_x(000) \left( 1 - e^{i(\frac{ka}{2\sqrt{2}})} \right) + u_z(000) \left( 1 - e^{i(\frac{ka}{2\sqrt{2}})} \right) \right] (\hat{i} + \hat{k}) \quad (65)$$

$$(66)$$