

Formulate the problem like this:

$$U_{harm} = \frac{1}{2} \sum_{\mathbf{R}, \mathbf{R}', u, v} \mathbf{u}_u(\mathbf{R}) D_{uv}(\mathbf{R} - \mathbf{R}') \mathbf{u}_v(\mathbf{R}'); \quad (1)$$

Work these out on paper:

$$D_{uv}(\mathbf{R} - \mathbf{R}') = \frac{\partial^2 U_{harm}}{\partial \mathbf{u}_u(\mathbf{R}) \partial \mathbf{u}_v(\mathbf{R}')} \quad (2)$$

Construct this:

$$D(\mathbf{k}) = \sum_{\mathbf{R}} D(\mathbf{R}) e^{-i\mathbf{k} \cdot \mathbf{R}} \quad (3)$$

Solve this:

$$M\omega^2 \epsilon = D(\mathbf{k}) \epsilon \quad (4)$$

The potential U_{harm} can be expressed in terms of displacements of atoms from their equilibrium positions $\mathbf{u}(\mathbf{R})$ and force constant matrices $D(\mathbf{R})$ which give the coupling between the atoms or cells. $D(\mathbf{k})$ is the $nd \times nd$ matrix we want to construct where n is the number of atoms in a unit cell and d is the spatial dimension. The aim is to solve the eigenvalue problem at each \mathbf{k} point. The band structure (ω_σ as a function of \mathbf{k}) is found by doing this for many \mathbf{k} points. The eigenvectors ϵ are indexed by σ which runs from 1 to nd . They are normal modes with frequency ω_σ . Being normal modes the motion of the system can always be expressed as a superposition of them and they are orthonormal. M is the mass which will be taken as a constant here but could of course vary for different atoms types.