# Normal modes of a three-dimensional harmonic crystal

Mike Hermele
(Dated: September 24, 2012)

To keep things simple, let's consider a monatomic 3d Bravais lattice. In that case, the general form of the Hamiltonian in the harmonic approximation is

$$H = \frac{1}{2M}\sum_{\boldsymbol{R}} \boldsymbol{p}_{\boldsymbol{R}}^2 + \frac{1}{2}\sum_{\boldsymbol{R},\boldsymbol{R}'} D^{\mu\nu}(\boldsymbol{R}-\boldsymbol{R}')u^{\mu}(\boldsymbol{R})u^{\nu}(\boldsymbol{R}'). \tag{1}$$

The matrix $D$ has the symmetry

$$D^{\mu\nu}(\boldsymbol{R}-\boldsymbol{R}') = D^{\nu\mu}(\boldsymbol{R}'-\boldsymbol{R}), \tag{2}$$

because it can be written as a second derivative

$$D^{\mu\nu}(\boldsymbol{R}-\boldsymbol{R}') = \left.\frac{\partial^2 U(\{\boldsymbol{R}+\boldsymbol{u}(\boldsymbol{R})\})}{\partial u^{\mu}(\boldsymbol{R})\partial u^{\nu}(\boldsymbol{R}')}\right|_{\boldsymbol{u}(\boldsymbol{R})=0}. \tag{3}$$

Also, any Bravais lattice has inversion symmetry, so $D^{\mu\nu}(\boldsymbol{R}) = D^{\mu\nu}(-\boldsymbol{R})$. Combining these two symmetries implies that $D^{\mu\nu}(\boldsymbol{R}) = D^{\nu\mu}(\boldsymbol{R})$ – that is, $D$ is a symmetric matrix.

As usual, we Fourier transform to find normal modes:

$$u^{\mu}(\boldsymbol{R}) = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}\in \text{B.Z.}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}u^{\mu}(\boldsymbol{k}) \tag{4}$$

$$u^{\mu}(\boldsymbol{k}) = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{R}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}u^{\mu}(\boldsymbol{R}). \tag{5}$$

Here, $N$ is the number of atoms in the crystal.

Note that $\boldsymbol{k}$ is restricted to lie in the 1st Brillouin Zone ("BZ") of the reciprocal lattice. (Note that very often we just say "Brillouin zone" and not "1st Brillouin zone.") To understand why this is so, suppose $\boldsymbol{k}' = \boldsymbol{k}+\boldsymbol{K}$, where $\boldsymbol{K}$ is a reciprocal lattice vector. Then, just as in the 1d case, we can show that $e^{i\boldsymbol{k}\cdot\boldsymbol{R}} = e^{i\boldsymbol{k}'\cdot\boldsymbol{R}}$. If $\boldsymbol{k}'$ is outside of the Brillouin zone, then there is a unique RLV $\boldsymbol{K}$ so that $\boldsymbol{k} = \boldsymbol{k}'-\boldsymbol{K}$ does lie inside the Brillouin zone. So we can restrict to $\boldsymbol{k}$ lying inside the Brillouin zone.

Another question is how many allowed values of $\boldsymbol{k}$ there are inside Brillouin zone – of course, this has to do with the periodic boundary conditions. Suppose $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$ are primitive vectors for the Bravais lattice. Suppose that the crystal has a size of $N_i$ lattice sites in the $\boldsymbol{a}_i$ direction, so that $\boldsymbol{R}, \boldsymbol{R}+N_1\boldsymbol{a}_1, \boldsymbol{R}+N_2\boldsymbol{a}_2, \boldsymbol{R}+N_3\boldsymbol{a}_3$ are all to be thought of as the same lattice site. (And also, the total number of atoms is $N = N_1N_2N_3$.) Next, suppose that $\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3$ are primitive vectors of the reciprocal lattice obtained from the $\boldsymbol{a}_i$ with the usual formula. A general allowed value of $\boldsymbol{k}$ can be written in the form

$$\boldsymbol{k} = \frac{n_1}{N_1}\boldsymbol{b}_1 + \frac{n_2}{N_2}\boldsymbol{b}_2 + \frac{n_3}{N_3}\boldsymbol{b}_3, \tag{6}$$

where $n_1, n_2, n_3$ are arbitrary integers. If we restrict $0 \le n_i \le N_i - 1$, then $\boldsymbol{k}$ is restricted to lie in the parallelepiped primitive cell defined by the $\boldsymbol{b}_i$. We can see that there are $N = N_1N_2N_3$ allowed values of $\boldsymbol{k}$ in this cell. The Brillouin zone has a different shape from this primitive cell, but it must contain the same number of allowed $\boldsymbol{k}$-values. So there are $N$ allowed values of $\boldsymbol{k}$ in the Brillouin zone. This is why we use the $1/\sqrt{N}$ normalization in Eqs. (4,5).

Plugging Eqs. ((4,5) into Eq. (1), we get

$$H = \frac{1}{2M}\sum_{\boldsymbol{k}\in \text{B.Z.}} \boldsymbol{p}_{\boldsymbol{k}}^{\dagger}\cdot\boldsymbol{p}_{\boldsymbol{k}} + \frac{1}{2}\sum_{\boldsymbol{k}\in \text{B.Z.}} D^{\mu\nu}(\boldsymbol{k})[u^{\mu}(\boldsymbol{k})]^{\dagger}u^{\nu}(\boldsymbol{k}), \tag{7}$$

where

$$D^{\mu\nu}(\boldsymbol{k}) = \frac{1}{N}\sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}D^{\mu\nu}(\boldsymbol{R}) \tag{8}$$

is a real, symmetric matrix. Because $D(\boldsymbol{k})$ is real and symmetric, it can be diagonalized by an orthogonal matrix $S(\boldsymbol{k})$:

$$S^\dagger(\boldsymbol{k})D(\boldsymbol{k})S(\boldsymbol{k}) = \mathrm{diag}(d_1(\boldsymbol{k}), d_2(\boldsymbol{k}), d_3(\boldsymbol{k})). \tag{9}$$

(Note that $S^\dagger = S^T = S^{-1}$, since $S$ is an orthogonal matrix.) We write

$$u^\mu(\boldsymbol{R}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k},\lambda} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} S_{\mu\lambda}(\boldsymbol{k}) u^\lambda(\boldsymbol{k}), \tag{10}$$

where we have introduced the index $\lambda = 1, 2, 3$ that runs over the three different phonon *polarizations*. The $u^\lambda(\boldsymbol{k})$ are the normal mode coordinates, each with frequency $\omega_\lambda(\boldsymbol{k}) = \sqrt{d_\lambda(\boldsymbol{k})/M}$.

To get a better feeling for the meaning of the $u^\lambda(\boldsymbol{k})$, the inverse Fourier transform is

$$u^\mu(\boldsymbol{k}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} u^\mu(\boldsymbol{R}) = S_{\mu\lambda}(\boldsymbol{k}) u^\lambda(\boldsymbol{k}). \tag{11}$$

Inverting this, we have

$$u^\lambda(\boldsymbol{k}) = S_{\mu\lambda}(\boldsymbol{k}) u^\mu(\boldsymbol{k}) = \frac{S_{\mu\lambda}(\boldsymbol{k})}{\sqrt{N}} \sum_{\boldsymbol{R}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} u^\mu(\boldsymbol{R}). \tag{12}$$

Because $S$ is an orthogonal matrix, its columns form an orthonormal basis. We use the symbol $\boldsymbol{s}_\lambda(\boldsymbol{k})$ to denote the column vectors of $S_{\mu\lambda}(\boldsymbol{k})$, which are labeled by the polarization $\lambda$. So we can finally write, for the normal mode coordinate:

$$u^\lambda(\boldsymbol{k}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} \big[\boldsymbol{s}_\lambda(\boldsymbol{k}) \cdot \boldsymbol{u}(\boldsymbol{R})\big]. \tag{13}$$

Basically, this equation means that $u^\lambda(\boldsymbol{k})$ describes a wave propagating along the $\boldsymbol{k}$-direction, where the displacement is always parallel to $\boldsymbol{s}_\lambda(\boldsymbol{k})$ everywhere along the wave, which is called the polarization vector.

In an isotropic medium there is no preferred direction, but when we are talking about a wave with wavevector $\boldsymbol{k}$, then $\boldsymbol{k}$ gives a preferred axis (about which there is rotational symmetry). So, in that case, we can always choose one of the $\boldsymbol{s}_\lambda(\boldsymbol{k})$ to be parallel to $\boldsymbol{k}$ – this is a longitudinally polarized wave. The other two are polarized perpendicular to $\boldsymbol{k}$, and are the transverse polarizations. The frequencies $\omega_\lambda(\boldsymbol{k})$ of the transverse polarizations are the same (by rotational symmetry about the $\boldsymbol{k}$-axis), but no symmetry (even in an isotropic medium!) dictates that the longitudinal and transverse modes need have the same frequency. Of course a crystal is not an isotropic medium, and usually the situation with polarizations is more complicated.

What we have found is that, in a 3d monatomic Bravais lattice, there are 3 different branches of normal modes, labeled by $\lambda$. This gives a total of $3N$ normal modes, which is what we expect for $3N$ atoms. Note that, here, having three branches comes simply from being in three dimensions and $\boldsymbol{u}, \boldsymbol{p}$ being vectors. By analogy with the 1d analysis, then, if we have a 3d lattice with basis, with $k$ sites per unit cell, we expect to have $3Nk$ branches of normal modes.

All of these three branches are acoustic phonons: they all must satisfy $\omega_\lambda(\boldsymbol{k}) \to 0$ for $\boldsymbol{k} \to 0$. The reason we have three modes with vanishing frequency is that there are now three independent overall translations of the whole crystal: $\boldsymbol{u}(\boldsymbol{R}) \to \boldsymbol{u}(\boldsymbol{R}) + \delta\boldsymbol{u}$, where $\delta\boldsymbol{u}$ is now an arbitrary vector. We can choose, for example, $\delta\boldsymbol{u} = \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$, and repeat the argument we gave in the 1d case for each one. So we expect three modes with vanishing frequency, and three acoustic branches.

It is very important to note that, in general, $\omega_\lambda(\boldsymbol{k}) = c_\lambda(\hat{\boldsymbol{k}})|\boldsymbol{k}|$ when $|\boldsymbol{k}|$ is small. So each of the acoustic modes has linear dispersion at small $\boldsymbol{k}$, and (for a given direction) propagates with a well-defined velocity. This is explained very clearly in Ashcroft & Mermin, and reading that discussion is highly recommended! The linear dispersion only relies on the interactions between atoms (*i.e.* $D^{\mu\nu}(\boldsymbol{R})$) being sufficiently short-ranged.