Symmetry

The basic symmetries of the dispersion

- The translational invariance of the lattice and reciprocal lattice.
- The point group symmetries of the lattice and reciprocal lattice.
- Time-reversal invariance.

Complex Properties of the dispersion and Eigenmodes

Due to the symmetric properties of the second derivative

$$D^{*\beta j}_{\alpha i} = \frac{1}{\sqrt{M_\alpha M_\beta}} \Phi^{0,\alpha,i}_{-p,\beta,j} e^{i\mathbf{q}\cdot(\mathbf{r}_p)} = \frac{1}{\sqrt{M_\alpha M_\beta}} \Phi^{p,\alpha,i}_{0,\beta,j} e^{i\mathbf{q}\cdot(\mathbf{r}_p)} = D^{\alpha i}_{\beta j}$$

Thus, $\boldsymbol{D}^{T} * = \boldsymbol{D}^{\dagger} = \boldsymbol{D}$ so $\boldsymbol{D}$ is hermitian and its eigenvalues ω^2 are real.

Suppose that the plane wave is moving to the right so that $\boldsymbol{q}=q_x$, then the plane of stationary phase travels to the right with $x = \dfrac{\omega}{q_x} t$

$$\xrightarrow{t \to -t} \quad \omega(-\mathbf{q}) = \omega(\mathbf{q})$$

$$\Rightarrow \quad D^{\alpha i}_{\beta j}(\mathbf{q}) = D^{*\alpha i}_{\beta j}(-\mathbf{q})$$

Return to the previous secular equation and associated orthogonality and completeness relations

$$\left(D^{\beta j}_{\alpha i}(\mathbf{q}) - \omega^2(\mathbf{q})\delta^{\beta j}_{\alpha i}\right)\epsilon_{\beta j}(\mathbf{q}) = 0$$

$$\sum_{\alpha,i}\epsilon^{*(n)}_{\alpha,i}(\mathbf{q})\epsilon^{(m)}_{\alpha,i}(\mathbf{q}) = \delta_{m,n} \quad \text{orthogonality}$$

$$\sum_{n}\epsilon^{*(n)}_{\alpha,i}(\mathbf{q})\epsilon^{*(n)}_{\beta,j}(\mathbf{q}) = \delta_{\alpha,\beta}\delta_{i,j}$$

Taking the complex conjugate of the secular equation

$$\left(D^{\beta j}_{\alpha i}(-\mathbf{q}) - \omega^2(-\mathbf{q})\delta^{\beta j}_{\alpha i}\right)\epsilon^{*}_{\beta j}(\mathbf{q}) = 0$$

$$\Rightarrow \quad \epsilon^{*}_{\beta j}(\mathbf{q}) = \epsilon_{\beta j}(-\mathbf{q})$$

Point-Group Symmetry and the Dispersion

From the definition of ***D***

$$D_{\alpha i}^{\beta j}(\mathsf{q}) = \frac{1}{\sqrt{M_\alpha M_\beta}} \Phi_{0\alpha i}^{p\beta j} e^{i\mathsf{q}\cdot(\mathsf{r}_p)}$$

and since $\boldsymbol{G}\cdot\boldsymbol{r}_p = 2\pi n$, (where n is an integer) it follows that

$$D_{\alpha i}^{\beta j}(\mathsf{q} + \mathsf{G}\ ) = D_{\alpha i}^{\beta j}(\mathsf{q})$$

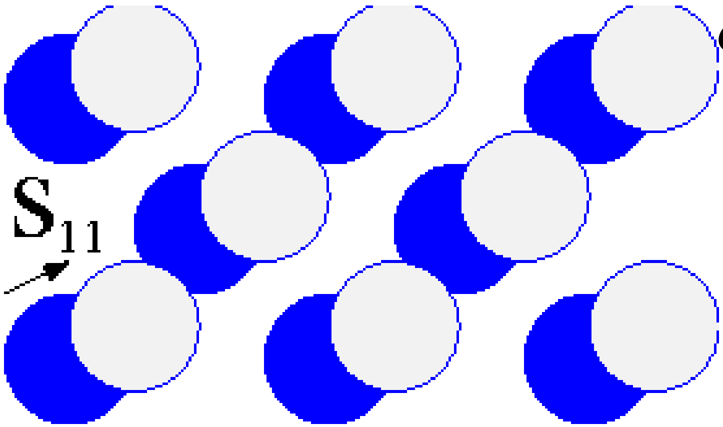
And in turn that the eigenvalues (and eigenvectors) must also be periodic.

$$\omega^{(n)}(\mathsf{k} + \mathsf{G}\ ) = \omega^{(n)}(\mathsf{k})$$

$$\epsilon_{\beta j}(\mathsf{k} + \mathsf{G}\ ) = \epsilon_{\beta j}(\mathsf{k})$$

Symmetry and the Need for Acoustic modes

Translational invariance



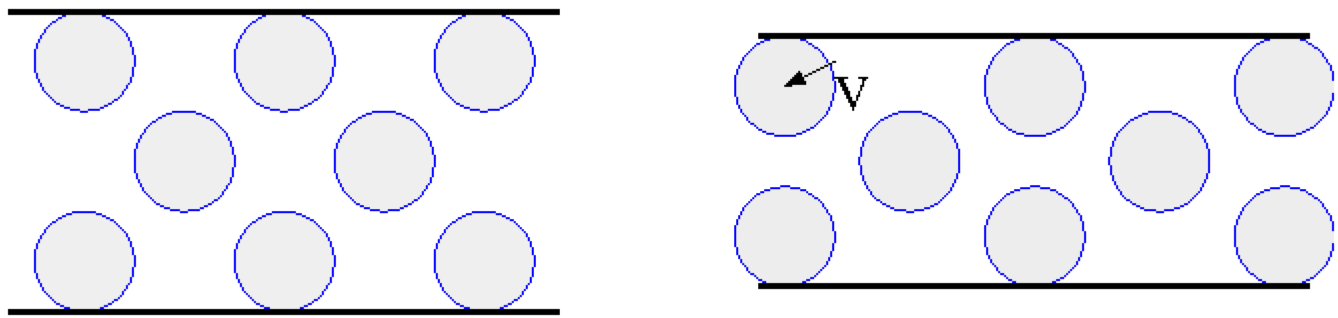
$$\begin{aligned} \delta E &= \frac{1}{2} \sum_{m,n,\alpha,\beta,i,j} \Phi_{0,\alpha,i}^{m-n,\beta,j} s_{n,\alpha,i} s_{m,\beta,j} = 0 \\ &= \frac{1}{2} \sum_{mn\alpha,\beta,i,j} \Phi_{0,\alpha,i}^{m-n,\beta,j} s_{1,1,i} s_{1,1,j} \\ &= \frac{1}{2} \sum_{i,j} s_{1,1,i} s_{1,1,j} \sum_{mn\alpha,\beta} \Phi_{0,\alpha,i}^{m-n,\beta,j} \end{aligned}$$

Since we know that $s_{1,1,i}$ is finite, it must be that

$$\sum_{m,n,\alpha,\beta} \Phi_{0,\alpha,i}^{m-n,\beta,j} = \sum_{p,\alpha,\beta} \Phi_{0,\alpha,i}^{p,\beta,j} = 0$$

Now consider a strain on the system $V_{m,\beta,j}$, described by the strain matrix *m*

$$V_{m,\beta,j} = \sum_{\alpha,i} m_{\beta,j}^{\alpha,i} s_{m,\alpha,i}$$



Net-force on the central (*n=0*) atom

$$0 = F_{0,\alpha,i} = -\sum_{m,\beta,j,\gamma,k} \Phi_{0,\alpha,i}^{m,\beta,j} m_{\beta,j}^{\gamma,k} s_{m,\gamma,k}$$

Since this applies for an arbitrary strain matrix *m* for each *m* must be zero

$$\Rightarrow \sum_{m} \Phi_{0,\alpha,i}^{m,\beta,j} s_{m,\gamma,k} = 0$$

The Counting of Modes

- Periodicity and the Quantization of States

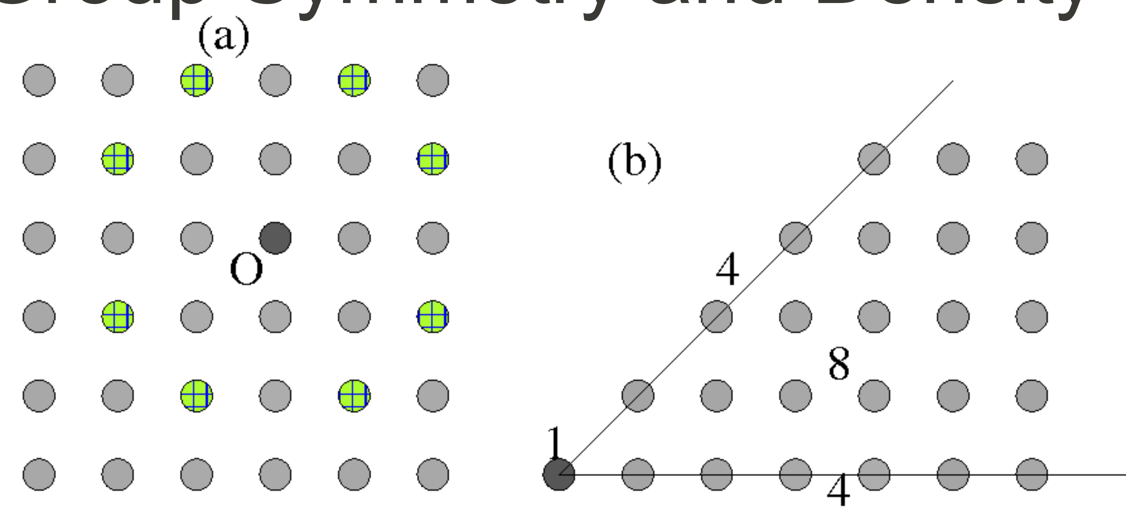
We were looking for solutions to the phonon problem of the form

$$s_n = \epsilon(q) e^{i(qr_n - \omega t)} \quad \text{where } r_n = na$$

Requiring $s_{n+N} = s_n$ or

$$q(n+N)a = qna + 2\pi m \quad \text{where } m \text{ is an integer}$$

- Translational Invariance: First Brillouin Zone
- Point Group Symmetry and Density of States



Normal Modes and Quantization

Any lattice displacement may be expressed as a sum over the eigen-vectors of the dynamical matrix D.

$$s_{n,\alpha,i} = \frac{1}{\sqrt{M_\alpha N}} \sum_{\mathbf{q},s} Q_s(\mathbf{q},t)\epsilon^s_{\alpha,i}(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}_n}$$

The kinetic energy of the lattice

$$\begin{aligned} T &= \frac{1}{2}\sum_{n,\alpha,i} M_\alpha \left(\dot{s}_{n\alpha,i}\right)^2 \\ &= \frac{1}{2N}\sum_{n,\alpha,i}\sum_{\mathbf{q},\mathbf{k},r,s} \dot{Q}_r(\mathbf{q})\epsilon^r_{\alpha,i}(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}_n}\dot{Q}_s(\mathbf{k})\epsilon^s_{\alpha,i}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}_n} \end{aligned}$$

Using $\frac{1}{N}\sum_n e^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{r}_n} = \delta_{\mathbf{k},-\mathbf{q}}$ and $\sum_{\alpha,i}\epsilon^r_{\alpha,i}\epsilon^{*s}_{\alpha,i} = \delta_{rs}$

$$\Rightarrow \quad T = \frac{1}{2}\sum_{\mathbf{q},r}\left|\dot{Q}_r(\mathbf{q})\right|^2$$

The potential energy may be rewritten in a similar fashion

$$V = \frac{1}{2} \sum_{n,m,\alpha,\beta,i,j} \Phi_{n,\alpha,i}^{m,\beta,j} s_{n,\alpha,i} s_{m,\beta,j}$$

$$= \frac{1}{2} \sum_{n,m,\alpha,\beta,i,j} \frac{\Phi_{0,\alpha,i}^{m-n,\beta,j}}{N\sqrt{M_\alpha M_\beta}} \sum_{\mathsf{q},\mathsf{k},s,r} Q_s(\mathsf{q},t)\epsilon_{\alpha,i}^{s}(\mathsf{q}) e^{i\mathsf{q}\cdot\mathsf{r}_n} Q_r(\mathsf{k},t)\epsilon_{\beta,j}^{r}(\mathsf{k}) e^{i\mathsf{k}\cdot\mathsf{r}_m}$$

Let $r_l = r_m - r_n$

$$V = \frac{1}{2} \sum_{n,l,\alpha,\beta,i,j} \frac{\Phi_{0,\alpha,i}^{l,\beta,j}}{N\sqrt{M_\alpha M_\beta}} \sum_{\mathsf{q},\mathsf{k},s,r} Q_s(\mathsf{q},t)\epsilon_{\alpha,i}^{s}(\mathsf{q}) e^{i\mathsf{q}\cdot\mathsf{r}_n} Q_r(\mathsf{k},t)\epsilon_{\beta,j}^{r}(\mathsf{k}) e^{i\mathsf{k}\cdot(\mathsf{r}_l+\mathsf{r}_n)}$$

and sum over n to obtain the delta function $\delta_{k,-q}$ so that

$$V = \frac{1}{2} \sum_{l,\alpha,\beta,i,j,s,r} Q_s(-\mathsf{k})\epsilon_{\alpha,i}^{s}(-\mathsf{k}) Q_r(\mathsf{k})\epsilon_{\beta,j}^{r}(\mathsf{k}) \frac{1}{\sqrt{M_\alpha M_\beta}} \Phi_{0,\alpha,i}^{l,\beta,j} e^{i\mathsf{k}\cdot\mathsf{r}_l}$$

This can be shown to reduce to

$$V = \frac{1}{2} \sum_{\mathsf{k},s} \omega_s^2(\mathsf{k}) \left| Q_s(\mathsf{k}) \right|^2$$

Thus we may write the Lagrangian of the ionic system as

$$L = T - V = \frac{1}{2} \sum_{\mathsf{k},s} \left(\left| \dot{Q}_s(\mathsf{k}) \right|^2 - \omega_s^2(\mathsf{k}) \left| Q_s(\mathsf{k}) \right|^2 \right)$$

where the $Q_s(\boldsymbol{k})$ may be regarded as canonical coordinates, and

$$P_r^*(\mathsf{k}) = \frac{\partial L}{\partial Q_r(\mathsf{k})} = \dot{Q}_s^*(\mathsf{k})$$

The equations of motion are

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{Q}_s^*(\mathsf{k})} \right) - \frac{\partial L}{\partial Q_s^*(\mathsf{k})} \quad \text{or} \quad \ddot{Q}_s(\mathsf{k}) + \omega_s^2(\mathsf{k}) Q_s(\mathsf{k}) = 0$$

Quantization and Second Quantization

1. First, identify the classical canonically conjugate set of variables $\{q_i, p_i\}$

2. These have Poisson Brackets

$$\{\{u,v\}\} = \sum_i \left(\frac{\partial u}{\partial q_i}\frac{\partial v}{\partial p_i} - \frac{\partial u}{\partial p_i}\frac{\partial v}{\partial q_i} \right)$$

$$\{\{q_i, p_j\}\} = \delta_{i,j} \quad \{\{p_i, p_j\}\} = \{\{q_i, q_j\}\} = 0$$

3. Then define the quantum Poisson Bracket (the commutator)

$$[u,v] = uv - vu = i\hbar\{\{u,v\}\}$$

4. In particular, $[q_i, p_j] = i\hbar\delta_{i,j}$, and $[q_i, q_j] = [p_i, p_j] = 0$

$\Rightarrow$ $[Q_r^*(\mathsf{k}), P_s(\mathsf{q})] = i\hbar\delta_{\mathsf{k},\mathsf{q}}\delta_{r,s}$ where the other commutators vanish .

Furthermore, since we have a system of *3rN* uncoupled harmonic oscillators we may immediately second quantize by introducing

$$
\begin{aligned}
a_s(\mathsf{k}) &= \frac{1}{\sqrt{2\hbar}}\left(\sqrt{\omega_s(\mathsf{k})}Q_s(\mathsf{k}) + \frac{i}{\sqrt{\omega_s(\mathsf{k})}}P_s(\mathsf{k})\right) \\
a_s^\dagger(\mathsf{k}) &= \frac{1}{\sqrt{2\hbar}}\left(\sqrt{\omega_s(\mathsf{k})}Q_s^*(\mathsf{k}) - \frac{i}{\sqrt{\omega_s(\mathsf{k})}}P_s^*(\mathsf{k})\right)
\end{aligned}
$$

Or,

$$
\begin{aligned}
Q_s(\mathsf{k}) &= \sqrt{\frac{\hbar}{2\omega_s(\mathsf{k})}}\left(a_s(\mathsf{k}) + a_s^\dagger(-\mathsf{k})\right) \\
P_s(\mathsf{k}) &= -i\sqrt{\frac{\hbar\omega_s(\mathsf{k})}{2}}\left(a_s(\mathsf{k}) - a_s^\dagger(-\mathsf{k})\right)
\end{aligned}
$$

Where

$$
[a_s(\mathsf{k}), a_r^\dagger(\mathsf{q})] = \delta_{r,s}\delta_{\mathsf{q},\mathsf{k}} \quad [a_s(\mathsf{k}), a_r(\mathsf{q})] = [a_s^\dagger(\mathsf{k}), a_r^\dagger(\mathsf{q})] = 0
$$

This transformation *{Q,P}* → *{a,a†}* is canonical, since is preserves the commutator algebra, and the Hamiltonian becomes

$$H = \sum_{k,s} \hbar\omega_s(\mathsf{k}) \left(a_s^\dagger(\mathsf{k}) a_s(\mathsf{k}) + \frac{1}{2} \right)$$

which is a sum over *3rN* independent quantum oscillators, each one referred to as a phonon mode!

The number of phonons in state *(k,s)*

$$n_s(\mathsf{k}) = a_s^\dagger(\mathsf{k}) a_s(\mathsf{k})$$

Phonon creation and destruction operators $a_s^\dagger(k)$ and $a_s(k)$

$$\begin{aligned} a_s^\dagger(\mathsf{k}) \left| n_s(\mathsf{k}) \right\rangle &= \sqrt{n_s(\mathsf{k}) + 1} \left| n_s(\mathsf{k}) + 1 \right\rangle \\ a_s(\mathsf{k}) \left| n_s(\mathsf{k}) \right\rangle &= \sqrt{n_s(\mathsf{k})} \left| n_s(\mathsf{k}) - 1 \right\rangle \end{aligned}$$

State with $\{n_s(k)\}$ phonons in each state *(k,s)* is

$$\left| \{ n_s(\mathsf{k}) \} \right\rangle = \left[\left(\prod_{\mathsf{k},s} \frac{1}{n_s(\mathsf{k})!} \right)^{\frac{1}{2}} \right] \prod_{\mathsf{k},s} \left(a_s^\dagger(\mathsf{k}) \right)^{n_s(\mathsf{k})} \left| 0 \right\rangle$$

The lattice point displacement:

$$s_{n,\alpha,i} = \frac{1}{\sqrt{M_\alpha N}} \sum_{\mathsf{q},s} \sqrt{\frac{\hbar}{2\omega_s(\mathsf{q})}} \left(a_s(\mathsf{q}) + a_s^\dagger(-\mathsf{q}) \right) \epsilon_{\alpha,i}^s(\mathsf{q}) e^{i\mathsf{q}\cdot\mathsf{r}_n}$$