

2. SYMMETRY ASPECTS OF EXCITATIONS

$\mathbf{D}_{\kappa\kappa'}$ ( $\mathbf{q}$ )	$3 \times 3$ submatrix of the dynamical matrix	$\mathbf{S}_-$	space-group element that inverts the wavevector
$\mathbf{D}_\alpha^i$	matrix of rotation about axis $i$ by the angle $\alpha$	$t$	time
$\mathbf{e}_\kappa(\mathbf{q}, j)$	polarization vector of atom $\kappa$ corresponding to the phonon ( $\mathbf{q}, j$ )	$T$	temperature
$\mathbf{e}(\mathbf{q}, j)$	eigenvector of the dynamical matrix corresponding to the phonon ( $\mathbf{q}, j$ )	$\mathbf{T}(\mathbf{q}, \mathbf{R})$ $= (T_{\kappa\kappa'}^{\alpha\mu}(\mathbf{q}, \mathbf{R}))$	matrix operator associated with a symmetry operation $\mathbf{r}$ of the point group of the wavevector $\mathbf{q}$
$E$	identity	$\mathbf{u}^o$	polarization vector for elastic waves
$\mathbf{E}(\mathbf{q}, s\alpha\lambda)$ $= (E_\kappa^\alpha(\mathbf{q}, s\alpha\lambda))$	matrix of symmetry coordinates	$\mathbf{u}_{\kappa l}(t)$	displacement vector of atom ( $\kappa l$ )
$E_o$	zero-point energy	$V$	potential energy
$E_{\text{ph}}$	lattice energy	$V$	volume
$E_{\mathbf{q}, j}$	contribution of the phonon ( $\mathbf{q}, j$ ) to the energy of the lattice	$\mathbf{V}(\kappa l, \kappa' l')$ $= (V_{\alpha\beta}(\kappa l, \kappa' l'))$	matrix of force constants acting between atoms ( $\kappa l$ ) and ( $\kappa' l'$ )
$f_o(\kappa, S)$	atom transformation table	$v_s$	sound velocity
$f_\sigma$	degeneracy of the eigenfrequency $\omega_{\mathbf{q}, \sigma}$	$\mathbf{v}(\mathbf{S})$	fractional translation associated with symmetry operation $\mathbf{S}$
$\mathbf{F}(\mathbf{q}) = (\mathbf{F}_{\kappa, \kappa'}(\mathbf{q}))$	Fourier-transformed force-constant matrix	$\mathbf{x}(m)$	lattice translation
$\mathbf{g}$	reciprocal-lattice vector	$Z$	partition function
$G(\mathbf{q})$	space group of the wavevector $\mathbf{q}$	$\boldsymbol{\alpha} = (\alpha_{\kappa l})$	tensor of thermal expansion
$G_o(\mathbf{q})$	point group of the wavevector $\mathbf{q}$	$\beta$	coefficient of volume expansion
$G_o(\mathbf{q}, -\mathbf{q})$	augmented point group of the wavevector $\mathbf{q}$	$\gamma$	mean Grüneisen parameter
$ G $	order of group $G$	$\gamma_{\mathbf{q}, j}$	averaged-mode Grüneisen parameter
$G(\omega)$	density of phonon states	$\gamma_{\mathbf{q}, \kappa l}$	generalized-mode Grüneisen parameters
$G^{\text{Debye}}(\omega)$	density of phonon states according to the Debye model	$\boldsymbol{\Gamma} = (\Gamma_{jl})$	propagation tensor
$G^{\text{Einstein}}(\omega)$	density of phonon states according to the Einstein model	$\boldsymbol{\Gamma} = (\Gamma_{\kappa\kappa'}^{\alpha\mu}(\mathbf{q}, \{\mathbf{S} \mathbf{v}(\mathbf{S}) + \mathbf{x}(m)\}))$	transformation matrix
$H$	Hamiltonian	$\delta_{\kappa l}$	Kronecker delta
$\hbar$	Planck constant ( $1.0546 \times 10^{-34}$ J s)	$\delta(\omega)$	Dirac delta function
$I$	inversion	$\Delta(\mathbf{q}, \mathbf{R})$	block-diagonal matrix of irreducible representations
$k$	Boltzmann constant ( $1.381 \times 10^{-23}$ J K $^{-1}$ )	$\boldsymbol{\varepsilon} = (\varepsilon_{\kappa l})$	strain tensor
$\mathbf{K}_o$	anti-unitary operator	$\chi$	character of a representation
$\mathbf{M}$	mass tensor	$\varphi(\mathbf{q}, \mathbf{r}_i, \mathbf{r}_j)$	multiplier associated with two symmetry operations $\mathbf{r}_i$ and $\mathbf{r}_j$ of the point group of the wavevector $\mathbf{q}$
$m_i$	mirror plane perpendicular to axis $i$	$\Phi$	potential energy
$m_\kappa$	mass of atom $\kappa$	$\kappa$	isothermal compressibility
$n_{\mathbf{q}, j}$	Bose factor corresponding to the phonon state ( $\mathbf{q}, j$ )	$\Theta_D$	Debye temperature
$N$	number of atoms within the primitive cell	$\Theta_E$	Einstein temperature
$N_Z$	number of primitive cells	$\rho$	density
$p$	pressure	$\boldsymbol{\sigma} = (\sigma_{\kappa l})$	stress tensor
$\mathbf{p}_{\kappa l}$	momentum of atom ( $\kappa l$ )	$\boldsymbol{\tau}^{(s)}(\mathbf{q}, \mathbf{R})$ $= (\tau_{\lambda\lambda'}^{(s)}(\mathbf{q}, \mathbf{R}))$	irreducible representation
$p_n$	occupation probability of quantum state $n$	$\overline{\boldsymbol{\tau}^{(s)}}(\mathbf{q}, \mathbf{R})$	conjugated representation
$\mathbf{P}^{(s)}(\mathbf{q}) = (P_{\lambda\lambda'}^{(s)}(\mathbf{q}))$	projection operator	$\boldsymbol{\tau}_v$	vector representation
$\mathbf{q}$	phonon wavevector	$\boldsymbol{\tau}_T$	tensor representation
$\mathbf{q}_{\text{BZ}}$	wavevector on the Brillouin-zone boundary	$\omega_D$	Debye frequency
$Q_{\mathbf{q}, j}$	normal coordinate corresponding to the phonon ( $\mathbf{q}, j$ )	$\omega_E$	Einstein frequency
$\mathbf{r}_l$	vector to the origin of the $l$ th primitive cell	$\omega_{\mathbf{q}, j}$	frequency of phonon ( $\mathbf{q}, j$ )
$\mathbf{r}_{\kappa l}(t)$	time-dependent position vector of atom ( $\kappa l$ )	$\boldsymbol{\Psi}$	arbitrary vector
$\mathbf{r}_\kappa^o$	equilibrium position of atom $\kappa$ with respect to the origin of the primitive cell	*	denotes the complex-conjugate quantity
$\mathbf{r}_{\kappa l}^o$	equilibrium position of atom $\kappa$ within the $l$ th primitive cell	+	denotes the Hermitian conjugate matrix
$\mathbf{R}$	element of the point group of the wavevector $G_o(\mathbf{q})$	$T$	denotes the transposed matrix
$\bar{\mathbf{R}}$	element of $G_o(\mathbf{q}, -\mathbf{q})$		
$\{\mathbf{S} \mathbf{v}(\mathbf{S}) + \mathbf{x}(m)\}$	symmetry operation (Seitz notation)		
$\mathbf{S} = (S_{\alpha\beta})$	matrix of rotation		

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## 2.1. PHONONS

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