GROUP-THEORETICAL ANALYSIS OF NORMAL VIBRATIONS OF THE Cu_2O CRYSTAL

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In this paper the group-theoretical methods and the results of Maradudin and Vosko are used to analyse the normal vibrations of the Cu_2O crystal. The Fourier-transformed dynamical matrices are reduced in analytic form for all symmetry points and lines in the Brillouin zone. Their eigenvalues and, whenever possible, the corresponding eigenvectors are given. Finally, the connectivity of the phonon dispersion relations is predicted.

1. Cu_2O lattice

The space structure of Cu_2O is illustrated in Fig. 1 [3]. Cu_2O has the space group $O_h^4(Pn3m)$. The lattice is simple cubic with six atoms per unit cell. The position vector of the equilibrium position of the $\varkappa$th atom in the lth unit cell is $\boldsymbol{x}(l\varkappa) = \boldsymbol{x}(l)+\boldsymbol{x}(\varkappa)$, where

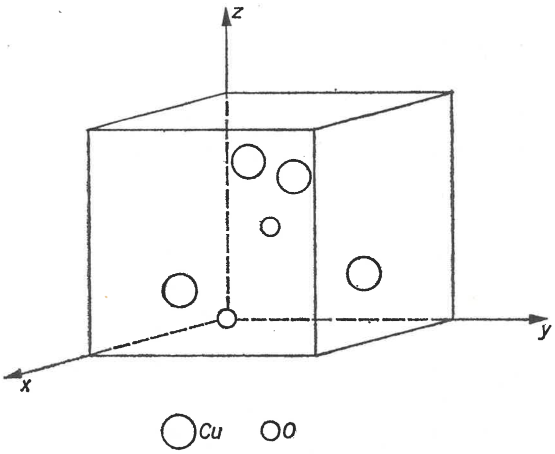

Fig. 1. Space structure of Cu_2O. Lattice constant $a = 4.252$ A

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$x(l)$ is the position vector of the origin of the lth unit cell and $x(\kappa)$ is the position vector of the κth kind of atom relative to the origin of the cell.

The position vectors $x(\kappa)$ for $\kappa = 1, 2, \ldots 6$ are as follows:

$$x(1) = (0, 0, 0),\ x(2) = (\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}),\ x(3) = (\tfrac{3}{4}, \tfrac{1}{4}, \tfrac{1}{4})$$

$$x(4) = (\tfrac{1}{4}, \tfrac{3}{4}, \tfrac{1}{4}),\ x(5) = (\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{3}{4}),\ x(6) = (\tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{4}).$$

We have assumed the lattice constant "a" as a unit. The isomorphic crystals to Cu_2O are the following: Ag_2O, Pb_2O, $Cd(CN)_2$ and $Zn(CN)_2$ [3].

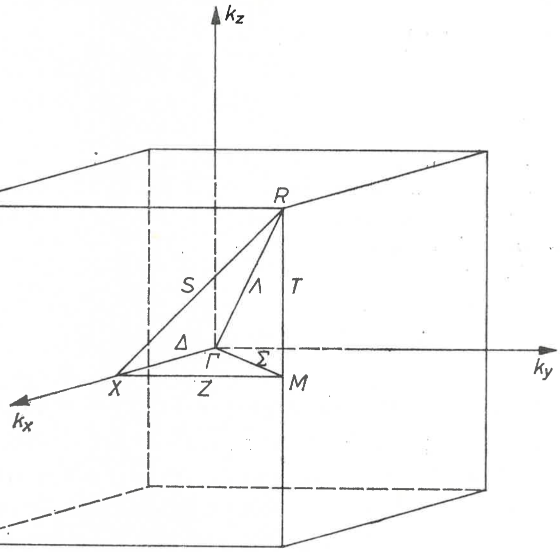

Fig. 2. The first Brillouin zone for the simple cubic lattice

In the reciprocal lattice the primitive vectors are the following: $k_x = (2\pi, 0, 0)$, $k_y = (0, 2\pi, 0)$ and $k_z = (0, 0, 2\pi)$. The first Brillouin zone for Cu_2O is shown in Fig. 2. The symmetry points and lines are equivalent respectively to the vectors:

$$\Gamma\text{-}\quad k = (0, 0, 0) \qquad \Sigma\text{-}\quad k = \pi(\xi, \xi, 0)$$

$$R\text{-}\quad k = (\pi, \pi, \pi) \qquad \Lambda\text{-}\quad k = \pi(\xi, \xi, \xi)$$

$$X\text{-}\quad k = (\pi, 0, 0) \qquad S\text{-}\quad k = \pi(1, \xi, \xi)$$

$$M\text{-}\quad k = (\pi, \pi, 0) \qquad T\text{-}\quad k = \pi(1, 1, \xi)$$

$$\Delta\text{-}\quad k = \pi(\xi, 0, 0) \qquad Z\text{-}\quad k = \pi(1, \xi, 0),$$

where $0 < \xi < 1$.

2. Procedure

The equations of motion of the crystal

$$M_\kappa \ddot{u}_\alpha(l\kappa) = -\partial\Phi/\partial u_\alpha(l\kappa) = -\sum_{l'\kappa'\beta} \Phi_{\alpha\beta}(l\kappa;\, l'\kappa')u_\beta(l'\kappa') \tag{1}$$

can be simplified to a set of $3r$ ("r" is the number of atoms per unit cell) equations in $3r$ unknowns by the substitution

$$u_\alpha(l\kappa) = [u_\alpha(\kappa)/(M_\kappa)^{\frac{1}{2}}] \exp[i\boldsymbol{k}\boldsymbol{x}(l) - i\omega t], \tag{2}$$

where M_κ is the mass of the κth kind of atom, $u_\alpha(l\kappa)$ is the α-Cartesian component of the displacement of the κth atom in the lth cell from its equilibrium position, $\boldsymbol{k}$ is the wave vector, Φ is the potential energy of the crystal, and $\Phi_{\alpha\beta}(l\kappa;\, l'\kappa')$ are the atomic force constants of the crystal. $\Phi_{\alpha\beta}(l\kappa;\, l'\kappa') = \partial^2\Phi/\partial u_\alpha(l\kappa)\, \partial u_\beta(l'\kappa')|_0$, where the subscript "0" indicates that the derivatives are evaluated in the configuration in which all atoms occupy their equilibrium positions.

When we substitute Eq. (2) into Eq. (1), the resulting equations for the amplitudes $\{u_\alpha(\kappa)\}$ can be written in the form:

$$\omega^2 u_\alpha(\kappa) = \sum_{\beta\kappa'} D_{\alpha\beta}(\kappa\kappa'|\boldsymbol{k})u_\beta(\kappa'), \qquad \alpha, \beta = x, y, z \quad \kappa, \kappa' = 1, 2, \ldots r, \tag{3}$$

where the elements of the $3r \times 3r$ matrix $\boldsymbol{D}(\boldsymbol{k})$, called the Fourier-transformed dynamical matrix, are given explicitly by

$$D_{\alpha\beta}(\kappa\kappa'|\boldsymbol{k}) = (M_\kappa M_{\kappa'})^{-\frac{1}{2}} \sum_{l'} \Phi_{\alpha\beta}(l\kappa;\, l'\kappa') \exp[-i\boldsymbol{k}(\boldsymbol{x}(l) - \boldsymbol{x}(l'))].$$

The condition for the set of homogeneous linear equations (3) to have nontrivial solutions for the amplitudes $\{u_\alpha(\kappa)\}$ is the vanishing of the determinant of the coefficients,

$$\det|\omega^2\delta_{\kappa\kappa'}\delta_{\alpha\beta} - D_{\alpha\beta}(\kappa\kappa'|\boldsymbol{k})| = 0. \tag{4}$$

For each value of $\boldsymbol{k}$, Eq. (4) has $3r$ solutions for ω^2. We display the dependence of ω on $\boldsymbol{k}$ explicitly, and label the solutions by an index j. The $\{\omega_j^2(\boldsymbol{k})\}$ are the eigenvalues of matrix $\boldsymbol{D}(\boldsymbol{k})$ and the $\{u_\alpha(\kappa)\}$ are the corresponding eigenvectors which we rewrite in the form $e_\alpha(\kappa|\boldsymbol{k}j)$ $(\boldsymbol{e}(\boldsymbol{k}j))$.

There are several properties of the dynamical matrix $\boldsymbol{D}(\boldsymbol{k})$, which are independent of the particular choice of $\boldsymbol{k}$. Some of these are listed below.

A. $\boldsymbol{D}(\boldsymbol{k})$ is Hermitian: $D_{\beta\alpha}(\kappa'\kappa|\boldsymbol{k}) = D_{\alpha\beta}(\kappa\kappa'|\boldsymbol{k})^*$

B. $\boldsymbol{D}(\boldsymbol{k}) = \boldsymbol{D}(-\boldsymbol{k})^*$

C. $\boldsymbol{D}(\boldsymbol{k})$ is periodic in the reciprocal lattice, *i. e.*
$\boldsymbol{D}(\boldsymbol{k}) = \boldsymbol{D}(\boldsymbol{k}+\boldsymbol{b})$, where $\boldsymbol{b}$ is the primitive vector.

For each of the symmetry points and lines we construct the multiplier representation $\{T(\boldsymbol{k};\, \mathscr{R})\}$:

$$T_{\alpha\beta}(\kappa\kappa'|\boldsymbol{k};\, \mathscr{R}) = \mathscr{R}_{\alpha\beta}\delta(\kappa, F_0(\kappa';\, \mathscr{R})) \exp\{i\boldsymbol{k}[\boldsymbol{x}(\kappa) - \mathscr{R}\boldsymbol{x}(\kappa')]\},$$

where $\{\mathscr{R}\}$ are the purely rotational elements in the space group G_k(taken by themselves, they comprise a point group of the vector $\boldsymbol{k}$), and κ is carried into $\bar{\kappa} = F_0(\kappa;\mathscr{R})$ by the operation $\{\mathscr{R}|\,\boldsymbol{v}(\mathscr{R})\}$:

$$\{\mathscr{R}|\,\boldsymbol{v}(\mathscr{R})\}\boldsymbol{x}(l\kappa) = \mathscr{R}\boldsymbol{x}(l\kappa)+\boldsymbol{v}(\mathscr{R}) = \mathscr{R}\boldsymbol{x}(l)+\mathscr{R}\boldsymbol{x}(\kappa)+\boldsymbol{v}(\mathscr{R}) = \boldsymbol{x}(\bar{l}\bar{\kappa}).$$

This multiplier representation has two significant uses. The first is based on the fact that all matrices in the representation commute with $\boldsymbol{D}(\boldsymbol{k})$. This gives an invariance condition

$$\boldsymbol{D}(\boldsymbol{k}) = \boldsymbol{T}(\boldsymbol{k};\mathscr{R})^{-1}\,\boldsymbol{D}(\boldsymbol{k})\,\boldsymbol{T}(\boldsymbol{k};\mathscr{R}). \tag{5}$$

If the point group of the crystal contains a rotational element $\mathscr{S}_-$ such that $\mathscr{S}_-\boldsymbol{k} = -\boldsymbol{k}$, we have the additional condition for matrix $\boldsymbol{D}(\boldsymbol{k})$:

$$\{\exp[-i\boldsymbol{k}\boldsymbol{x}(\bar{\kappa})]D_{\mu\nu}(\bar{\kappa}\bar{\kappa}'|\boldsymbol{k})\exp[i\boldsymbol{k}\boldsymbol{x}(\bar{\kappa}')]\}^* =$$
$$= \sum_{\alpha\beta}(\mathscr{S}_-)_{\mu\alpha}\{\exp[-i\boldsymbol{k}\boldsymbol{x}(\kappa)]D_{\alpha\beta}(\kappa\kappa'|\boldsymbol{k})\exp[i\boldsymbol{k}\boldsymbol{x}(\kappa')]\}(\mathscr{S}_-)_{\nu\beta}, \tag{6}$$

where $\bar{\kappa}$ and $\bar{\kappa}'$ are the labels of the atoms into which the atoms κ and κ' are sent by the operation $\{\mathscr{S}_-|\,\boldsymbol{v}(\mathscr{S}_-)\}$. The second use of $\{\boldsymbol{T}(\boldsymbol{k};\mathscr{R})\}$ is in the construction of symmetry--adapted eigenvectors $\boldsymbol{E}(\boldsymbol{k};s\lambda)$.

We use the decomposition formula

$$c_s = h^{-1}\sum_{\mathscr{R}}\chi(\boldsymbol{k};\mathscr{R})\chi^{(s)}(\boldsymbol{k};\mathscr{R})^*$$

to find how many times the irreducible multiplier representation $\{\boldsymbol{\tau}^{(s)}(\boldsymbol{k};\mathscr{R})\}$ is contained in $\{\boldsymbol{T}(\boldsymbol{k};\mathscr{R})\}$. The order of the point group of the wave vector is h. $\chi(\boldsymbol{k};\mathscr{R})$ and $\chi^{(s)}(\boldsymbol{k};\mathscr{R})$ are the characters of the matrices $\boldsymbol{T}(\boldsymbol{k};\mathscr{R})$ and $\boldsymbol{\tau}^{(s)}(\boldsymbol{k};\mathscr{R})$, respectively.

The transformation properties of $\boldsymbol{E}(\boldsymbol{k};s\lambda)$ are defined by the equation

$$\boldsymbol{T}(\boldsymbol{k};\mathscr{R})\boldsymbol{E}(\boldsymbol{k};s\lambda) = \sum_{\lambda'}\tau^{(s)}_{\lambda'\lambda}(\boldsymbol{k};\mathscr{R})\boldsymbol{E}(\boldsymbol{k};s\lambda').$$

$\boldsymbol{E}(\boldsymbol{k};s\lambda)$ is obtained by use of projection operators $\boldsymbol{P}^{(s)}_{\lambda\lambda'}(\boldsymbol{k})$:

$$\boldsymbol{E}(\boldsymbol{k};s\lambda) = \boldsymbol{P}^{(s)}_{\lambda\lambda'}(\boldsymbol{k})\psi,$$

where ψ is an arbitrary $3r$-dimensional column matrix, and

$$\boldsymbol{P}^{(s)}_{\lambda\lambda'}(\boldsymbol{k}) = (f_s/h)\sum_{\mathscr{R}}\tau^{(s)}_{\lambda\lambda'}(\boldsymbol{k};\mathscr{R})^*\boldsymbol{T}(\boldsymbol{k};\mathscr{R}),$$

where f_s is the dimension of the sth irreducible representation.

When $c_s \leqslant 2$, these vectors will be substituted into the eigenvalue equation:

$$\boldsymbol{D}(\boldsymbol{k})\boldsymbol{E}(\boldsymbol{k};s\lambda) = \omega^2_{sa}(\boldsymbol{k})\boldsymbol{E}(\boldsymbol{k};s\lambda)$$

and the orthonormal eigenvectors $\boldsymbol{e}(\boldsymbol{k}sa\lambda)$ will be written out explicitly. Now we replace the simple index j by $sa\lambda$, where "a" is the "repetition" index which differentiates among the different eigenvalues, whose associated eigenvectors transform according to the same irreducible sth representation of the point group $G_0(\boldsymbol{k})$ of the wave vector $\boldsymbol{k}$. The index "a" takes on the values 1, 2, ... c_s. For $c_s > 2$, only the determinant condition for branches belonging to $\tau^{(s)}$ is recorded.

Time-reversal symmetry can produce extra degeneracies in the lattice vibration frequencies. The test criteria for irreducible representations which belong to one of the three types are presented in [1].

3. *Application of the procedure to the Cu_2O crystal*

In this part we give the simplified (Eqs (5) and (6)) analytic form of $\boldsymbol{D}(\boldsymbol{k})$ and the corresponding eigenvectors (polarization vectors) and eigenvalues.

If the irreducible multiplier representation $\{\tau^{(s)}(\boldsymbol{k}; \mathcal{R})\}$ is contained in $\{\boldsymbol{T}(\boldsymbol{k}; \mathcal{R})\}$ more than twice, we shall give only the matrix $\boldsymbol{D}_s(\boldsymbol{k})$. Equation det $(\boldsymbol{D}_s(\boldsymbol{k}) - \boldsymbol{1}\omega^2_{sa}(\boldsymbol{k}) = 0$ is the determinant condition for the eigenvalues. We also give the linear combination $\boldsymbol{E}(\boldsymbol{k}; s\lambda)$ of the corresponding eigenvectors transforming accordingly to $\{\tau^{(s)}(\boldsymbol{k}, \mathcal{R})\}$.

The matrices $\boldsymbol{D}_s(\boldsymbol{k})$ are obtained by using the unitary transformation

$$\boldsymbol{U}^{-1}\boldsymbol{D}(\boldsymbol{k})\,\boldsymbol{U} = \begin{bmatrix} \ddots & & \\ & \boldsymbol{D}_s(\boldsymbol{k}) & \\ & & \ddots \end{bmatrix},$$

where the columns of the unitary matrix $\boldsymbol{U}$ are either the eigenvectors of $\boldsymbol{D}(\boldsymbol{k})$ or vectors whose linear combinations form $\boldsymbol{E}(\boldsymbol{k}; s\lambda)$.

When the requirement is to calculate the eigenvectors $\boldsymbol{e}(\boldsymbol{k}sa\lambda)$ from $\boldsymbol{E}(\boldsymbol{k}; s\lambda)$, the following possibility is available.

Multiplication of the vector $\boldsymbol{E}(\boldsymbol{k}; s\lambda)$ by the matrix $\boldsymbol{D}(\boldsymbol{k})$ yields c_s complex homogeneous equations in c_s unknown complex components of this vector; this suffices to determine the c_s eigenvectors $\boldsymbol{e}(\boldsymbol{k}sa\lambda)$. Since the equations are homogeneous, one must find the solution $2(c_s-1)$ real quantities and then normalize the eigenvector to unity. One can reduce the number of unknown real quantities in $\boldsymbol{E}(\boldsymbol{k}; s\lambda)$ from $2(c_s-1)$ to (c_s-1) when $c_s > 1$. In order to make this possible, the conditions

$$\boldsymbol{e}(\boldsymbol{k}sa\lambda) = \boldsymbol{e}^*\boldsymbol{k}\, sa\lambda)$$

for $\boldsymbol{k}$ equivalent to the symmetry points, and

$$e^*_\alpha(2|\boldsymbol{k}sa\lambda) = \exp\left[-i\boldsymbol{k}\boldsymbol{x}(2)\right]e_\alpha(1|\boldsymbol{k}sa\lambda)$$

$$e^*_\alpha(\kappa|\boldsymbol{k}sa\lambda) = \exp\left[-2i\boldsymbol{k}\boldsymbol{x}(\kappa)\right]e_\alpha(\kappa|\boldsymbol{k}sa\lambda),$$

where

$$\alpha = x, y, z.$$

$$\kappa = 3, 4, 5, 6,$$

for $\boldsymbol{k}$ equivalent to the symmetry lines, may be introduced. (The vector $\boldsymbol{e}(\boldsymbol{k}j)$ in component form is $\boldsymbol{e}^T(\boldsymbol{k}j) = (e_x(1|\boldsymbol{k}j), e_y(1|\boldsymbol{k}j), e_z(1|\boldsymbol{k}j), e_x(2|\boldsymbol{k}j), \ldots))$. Since it is convenient to present vector components in the form of a row rather than a column, we shall write down the

TABLE I

Irreducible multiplier representations of the groups $G_0(\boldsymbol{k})$

Point	$G_0(\boldsymbol{k})$	Representations
Γ	$m3m$	$\Gamma_4 = \tau^4$ $\Gamma_7 = \tau^{2(-)}$ $\Gamma_8 = \tau^{3(-)}$, $\Gamma_9 = \tau^{4(-)}$ $\Gamma_{10} = \tau^{5(-)}$
R	$m3m$	$R_4 = \tau^4$ $R_7 = \tau^{2(-)}$ $R_8 = \tau^{3(-)}$, $R_9 = \tau^{4(-)}$ $R_{10} = \tau^{5(-)}$
X	$4/mmm$	(see below)
M	$4/mmm$	$M_1 = \tau^1$ $M_2 = \tau^2$ $M_3 = \tau^3$, $M_4 = \tau^4$,
Line		
Δ	$4mm$	(see below)

X, $4/mmm$:

	h_1	h_2	h_3	h_4	h_{17}	h_{18}	h_{19}	h_{20}	h_{25}	h_{26}	h_{27}	h_{28}	h_{41}	h_{42}	h_{43}	h_{44}
X_1	σ_0	$-\sigma_0$	$-\sigma_x$	σ_x	$-i\sigma_0$	$i\sigma_0$	$-i\sigma_x$	$i\sigma_x$	$i\sigma_z$	$-i\sigma_z$	σ_y	$-\sigma_y$	$-\sigma_z$	σ_z	$-i\sigma_y$	$i\sigma_y$
X_2	σ_0	$-\sigma_0$	σ_x	$-\sigma_x$	$i\sigma_0$	$-i\sigma_0$	$-i\sigma_x$	$i\sigma_x$	$i\sigma_z$	$-i\sigma_z$	$-\sigma_y$	σ_y	σ_z	$-\sigma_z$	$-i\sigma_y$	$i\sigma_y$
X_3	σ_0	σ_0	σ_x	σ_x	$i\sigma_z$	$i\sigma_z$	$-\sigma_y$	$-\sigma_y$	$i\sigma_z$	$i\sigma_z$	$-\sigma_y$	$-\sigma_y$	σ_0	σ_0	σ_x	σ_x
X_4	σ_0	σ_0	σ_x	σ_x	$-i\sigma_z$	$-i\sigma_z$	σ_y	σ_y	$i\sigma_z$	$i\sigma_z$	$-\sigma_y$	$-\sigma_y$	$-\sigma_0$	$-\sigma_0$	$-\sigma_x$	$-\sigma_x$

Δ, $4mm$:

	h_1	h_2	h_{19}	h_{20}	h_{27}	h_{28}	h_{41}	h_{42}
Δ_1	1	1	1	1	1	1	1	1
Δ_2	1	1	1	1	−1	−1	−1	−1
Δ_3	1	1	−1	−1	1	1	−1	−1
Δ_4	1	1	−1	−1	−1	−1	1	1
Δ_5	σ_0	$-\sigma_0$	$-i\sigma_y$	$i\sigma_y$	σ_z	$-\sigma_z$	$-\sigma_x$	σ_z

T	$4mm$	$T_\alpha = \tau^\alpha$ for $\alpha = 1, 2, 3, 4.$; $T_5 = \tau^{5'}$				
Λ	$3m$	$\Lambda_\alpha = \tau^\alpha$ for $\alpha = 1, 2.$; $\Lambda_3 = \tau^{3'}$				
Σ	$mm2$	$\Sigma_\alpha = \tau^\alpha$				
S	$mm2$		h_1	h_{18}	h_{26}	h_{41}
		S_1	1	i	i	1
		S_2	1	$-i$	$-i$	1
		S_3	1	$-i$	i	-1
		S_4	1	i	$-i$	-1
Z	$mm2$		h_1	h_3	h_{26}	h_{28}
		Z_1	σ_0	$-\sigma_y$	$-i\sigma_z$	σ_x

h is the $\mathscr{R}$ — Kovalev's rotational element and τ is Kovalev's irreducible multiplier representation.
$\tau' = U\tau U^{-1}$, where the unitary matrices U are as follows:

$$U = \frac{1}{\sqrt{2}}\begin{bmatrix} \exp\left(i\frac{\pi}{4}\right), & \exp\left(i\frac{\pi}{4}\right) \\ -\exp\left(-i\frac{\pi}{4}\right), & \exp\left(-i\frac{\pi}{4}\right) \end{bmatrix} \text{ for } \Gamma_8, R_8, \Lambda_3 \text{ and } U = \frac{1}{\sqrt{2}}\begin{bmatrix} 1, & -i \\ -i, & 1 \end{bmatrix} \text{ for } M_3, M_4, T_5.$$

σ_α are the Pauli spin matrices: $\sigma_0 = \begin{bmatrix} 1, & 0 \\ 0, & 1 \end{bmatrix}$, $\sigma_x = \begin{bmatrix} 0, & 1 \\ 1, & 0 \end{bmatrix}$,

$$\sigma_y = \begin{bmatrix} 0, & -i \\ i, & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1, & 0 \\ 0, & -1 \end{bmatrix}.$$

TABLE II

Decomposition of the representation $\{T(k;\mathscr{R})\}$ for all symmetry points and lines in the Brillouin zone of the Cu_2O lattice

Point Γ	$\Gamma_4 \oplus \Gamma_7 \oplus \Gamma_8 \oplus \Gamma_9 \oplus 3\Gamma_{10}$
R	$R_4 \oplus R_7 \oplus R_8 \oplus R_9 \oplus 3R_{10}$
X	$2X_1 \oplus 3X_2 \oplus 3X_3 \oplus X_4$
M	$2M_1 \oplus 3M_2 \oplus M_3 \oplus 3M_4$
Line Δ	$3\Delta_1 \oplus \Delta_2 \oplus \Delta_3 \oplus 3\Delta_4 \oplus 5\Delta_5$
T	$3T_1 \oplus T_2 \oplus T_3 \oplus 3T_4 \oplus 5T_5$
Λ	$5\Lambda_1 \oplus \Lambda_2 \oplus 6\Lambda_3$
Σ	$5\Sigma_1 \oplus 3\Sigma_2 \oplus 4\Sigma_3 \oplus 6\Sigma_4$
S	$5S_1 \oplus 6S_2 \oplus 4S_3 \oplus 3S_4$
Z	$9Z_1$

TABLE III

Compatibility relations

Point Γ	Δ	Σ	Λ
Γ_4	$\Delta_4 \oplus \Delta_5$	$\Sigma_1 \oplus \Sigma_2 \oplus \Sigma_4$	$\Lambda_1 \oplus \Lambda_3$
Γ_7	Δ_4	Σ_4	Λ_1
Γ_8	$\Delta_2 \oplus \Delta_4$	$\Sigma_2 \oplus \Sigma_4$	Λ_3
Γ_9	$\Delta_3 \oplus \Delta_5$	$\Sigma_1 \oplus \Sigma_2 \oplus \Sigma_3$	$\Lambda_2 \oplus \Lambda_3$
Γ_{10}	$\Delta_1 \oplus \Delta_5$	$\Sigma_1 \oplus \Sigma_3 \oplus \Sigma_4$	$\Lambda_1 \oplus \Lambda_3$

Point R	Λ	S	T
R_4	$\Lambda_1 \oplus \Lambda_3$	$S_1 \oplus S_2 \oplus S_4$	$T_4 \oplus T_5$
R_7	Λ_1	S_2	T_4
R_8	Λ_3	$S_2 \oplus S_4$	$T_2 \oplus T_4$
R_9	$\Lambda_2 \oplus \Lambda_3$	$S_1 \oplus S_3 \oplus S_4$	$T_3 \oplus T_5$
R_{10}	$\Lambda_1 \oplus \Lambda_3$	$S_1 \oplus S_2 \oplus S_3$	$T_1 \oplus T_5$

Point X	Δ	S	Z
X_1	Δ_5	$S_1 \oplus S_4$	Z_1
X_2	Δ_5	$S_2 \oplus S_3$	Z_1
X_3	$\Delta_1 \oplus \Delta_4$	$S_1 \oplus S_2$	Z_1
X_4	$\Delta_2 \oplus \Delta_3$	$S_3 \oplus S_4$	Z_1

Point M	Σ	T	Z
M_1	$\Sigma_1 \oplus \Sigma_2$	T_5	Z_1
M_2	$\Sigma_3 \oplus \Sigma_4$	T_5	Z_1
M_3	$\Sigma_2 \oplus \Sigma_3$	$T_2 \oplus T_3$	Z_1
M_4	$\Sigma_1 \oplus \Sigma_4$	$T_1 \oplus T_4$	Z_1

transposed vectors as $e^T(k\ sa\lambda)$ and $E^T(k;s\lambda)$. Finally, we present the possible arrangement of dispersion curves for Cu_2O (Fig. 3). The plots in Fig. 3 are found on the basis of compatibility relations given in Table III and the assumption that crossing branches belonging to the same representation are unlikely [2].

Furthermore, we know that there are three acoustic branches (longitudinal-acoustic LA or transverse-acoustic TA) of the dispersion relation along each of the symmetry lines

$\Delta_1\Sigma$ and Λ. We can see from the explicit form of the eigenvectors that the acoustic branches belong to the representations Δ_1, Δ_5 along Δ, $\Sigma_1, \Sigma_3, \Sigma_4$ along Σ and Λ_1, Λ_3 along Λ.

Bearing this in mind, we can see that at Γ one of the eigenvalues belonging to the representation Γ_{10} is equal to zero. The irreducible multiplier representations and the

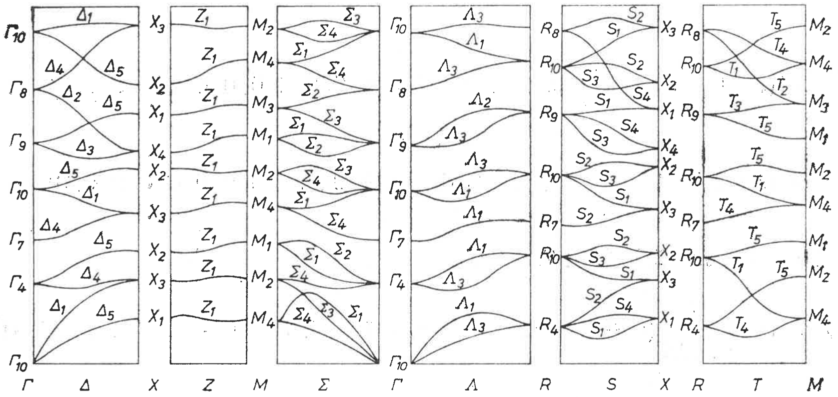

Fig. 3. Possible arrangement of dispersion curves for Cu_2O obtained by group theory. No physical data has been used

decompositions of the representations are given in Tables I and II. The time-reversal symmetry does not produce any additional degeneracy at any point or line.

The author wishes to thank Professor M. Suffczyński for suggesting the present investigation as well as for his advice and critical remarks.

Symmetry at Γ

$$D(\Gamma)=\begin{bmatrix}
A & O & O & B & O & O & C & D & D & C & D & -D & C & -D & D & C & -D & -D \\
O & A & O & O & B & O & D & C & -D & D & C & D & -D & C & D & -D & C & -D \\
O & O & A & O & O & B & D & -D & C & -D & D & C & D & D & C & -D & -D & C \\
B & O & O & A & O & O & C & D & D & C & D & -D & C & -D & D & C & -D & -D \\
O & B & O & O & A & O & D & C & -D & D & C & D & -D & C & D & -D & C & -D \\
O & O & B & O & O & A & D & -D & C & -D & D & C & D & D & C & -D & -D & C \\
C & D & D & C & D & D & E & F & F & G & J & K & G & K & J & H & -K & -K \\
D & C & -D & D & C & -D & F & E & -F & J & G & -K & -K & H & K & K & G & -J \\
D & -D & C & D & -D & C & F & -F & E & -K & K & H & J & -K & G & K & -J & G \\
C & D & -D & C & D & -D & G & J & -K & E & F & -F & H & -K & K & G & K & -J \\
D & C & D & D & C & D & J & G & K & F & E & F & K & G & J & -K & H & -K \\
-D & D & C & -D & D & C & K & -K & H & -F & F & E & -K & J & G & -J & K & G \\
C & -D & D & C & -D & D & G & -K & J & H & K & -K & E & -F & F & G & -J & K \\
-D & C & D & -D & C & D & K & H & -K & -K & G & J & -F & E & F & -J & G & K \\
D & D & C & D & D & C & J & K & G & K & J & G & F & F & E & -K & -K & H \\
C & -D & -D & C & -D & -D & H & K & K & G & -K & -J & G & -J & -K & E & -F & -F \\
-D & C & -D & -D & C & -D & -K & G & -J & K & H & K & -J & G & -K & -F & E & -F \\
-D & -D & C & -D & -D & C & -K & -J & G & -J & -K & G & K & K & H & -F & -F & E
\end{bmatrix}$$

$D(\Gamma)$ is real. The number of independent elements of $D(\Gamma)$ is equal 10.

The eigenvalues and eigenvectors of $\boldsymbol{D}(\Gamma)$:

$\omega^2_{4,1}(\Gamma) = A-B$ (threefold degenerate)

$$\boldsymbol{e}^T(\Gamma; 4, 1, 1) = \frac{1}{\sqrt{2}}(1, 0, 0, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

$$\boldsymbol{e}^T(\Gamma; 4, 1, 2) = \frac{1}{\sqrt{2}}(0, 1, 0, 0, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

$$\boldsymbol{e}^T(\Gamma; 4, 1, 3) = \frac{1}{\sqrt{2}}(0, 0, 1, 0, 0, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

$\omega^2_{7,1}(\Gamma) = E+H-2F-2G+2J-4K$

$$\boldsymbol{e}^T(\Gamma; 7, 1, 1) = \frac{1}{2\sqrt{3}}(0, 0, 0, 0, 0, 0, 1, -1, -1, -1, 1, -1, -1, -1, 1, 1, 1, 1)$$

$\omega^2_{8,1}(\Gamma) = E+F+H-J-2G+2K$ (twofold degenerate)

$$\boldsymbol{e}^T(\Gamma; 8, 1, 1) = \frac{1}{2\sqrt{2}}(0, 0, 0, 0, 0, 0, 1, 1, 0, -1, -1, 0, -1, 1, 0, 1, -1, 0)$$

$$\boldsymbol{e}^T(\Gamma; 8, 1, 2) = \frac{1}{2\sqrt{6}}(0, 0, 0, 0, 0, 0, 1, -1, 2, -1, 1, 2, -1, -1, -2, 1, 1, -2)$$

$\omega^2_{9,1}(\Gamma) = E+F-H-J-2K$ (threefold degenerate)

$$\boldsymbol{e}^T(\Gamma; 9, 1, 1) = \frac{1}{2\sqrt{2}}(0, 0, 0, 0, 0, 0, 0, 1, -1, 0, 1, 1, 0, -1, -1, 0, -1, 1)$$

$$\boldsymbol{e}^T(\Gamma; 9, 1, 2) = \frac{1}{2\sqrt{2}}(0, 0, 0, 0, 0, 0, -1, 0, -1, -1, 0, 1, 1, 0, 1, 1, 0, -1)$$

$$\boldsymbol{e}^T(\Gamma; 9, 1, 3) = \frac{1}{2\sqrt{2}}(0, 0, 0, 0, 0, 0, 1, 1, 0, -1, -1, 0, 1, -1, 0, -1, 1, 0)$$

$$\boldsymbol{D}_{10}(\Gamma) = \begin{bmatrix} A+B & 2\sqrt{2}C & 4D \\ 2\sqrt{2}C & E+H+2G & \sqrt{2}(F+J) \\ 4D & \sqrt{2}(F+J) & E-F-H+J+2K \end{bmatrix}$$

Each eigenvalue of $\boldsymbol{D}_{10}(\Gamma)$ is threefold degenerate and one of them is equal zero.

$\boldsymbol{E}^T(\Gamma; 10, 1) = (a,\ 0,\ 0,\ a,\ 0,\ 0,\ b,\ c,\ c,\ b,\ c,\ -c,\ b,\ -c,\ c,\ b,\ -c,\ -c)$

$\boldsymbol{E}^T(\Gamma; 10, 2) = (0,\ a,\ 0,\ 0,\ a,\ 0,\ c,\ b,\ -c,\ c,\ b,\ c,\ -c,\ b,\ c,\ -c,\ b,\ -c)$

$\boldsymbol{E}^T(\Gamma; 10, 3) = (0,\ 0,\ a,\ 0,\ 0,\ a,\ c,\ -c,\ b,\ -c,\ c,\ b,\ c,\ c,\ b,\ -c,\ -c,\ b)$

Symmetry at R

$$
D(R) = \begin{bmatrix}
A & 0 & 0 & -B & 0 & 0 & C & D & D & C & D & -D & C & -D & D & C & -D & -D \\
0 & A & 0 & 0 & -B & 0 & D & C & -D & D & C & D & -D & C & D & -D & C & -D \\
0 & 0 & A & 0 & 0 & -B & D & -D & C & -D & D & C & D & D & C & -D & -D & C \\
-B & 0 & 0 & A & 0 & 0 & -C & -D & -D & -C & -D & D & -C & D & -D & -C & D & D \\
0 & -B & 0 & 0 & A & 0 & -D & -C & D & -D & -C & -D & D & -C & -D & D & -C & D \\
0 & 0 & -B & 0 & 0 & A & -D & D & -C & D & -D & -C & -D & -D & -C & D & D & -C \\
C & D & D & -C & -D & -D & E & F & F & G & J & K & G & K & J & H & -K & -K \\
D & C & -D & -D & -C & D & F & E & -F & J & G & -K & -K & H & K & K & G & -J \\
D & -D & C & -D & D & -C & F & -F & E & -K & K & H & J & -K & G & K & -J & G \\
C & D & -D & -C & -D & D & G & J & -K & E & F & -F & H & -K & K & G & K & -J \\
D & C & D & -D & -C & -D & J & G & K & F & E & F & K & G & J & -K & H & -K \\
-D & D & C & D & -D & -C & K & -K & H & -F & F & E & -K & J & G & -J & K & G \\
C & -D & D & -C & D & -D & G & -K & J & H & K & -K & E & -F & F & G & -J & K \\
-D & C & D & D & -C & -D & K & H & -K & -K & G & J & -F & E & F & -J & G & K \\
D & D & C & -D & -D & -C & J & K & G & K & J & G & F & F & E & -K & -K & H \\
C & -D & -D & -C & D & D & H & K & K & G & -K & -J & G & -J & -K & E & -F & -F \\
-D & C & -D & D & -C & D & -K & G & -J & K & H & K & -J & G & -K & -F & E & -F \\
-D & -D & C & D & D & -C & -K & -J & G & -J & -K & G & K & K & H & -F & -F & E
\end{bmatrix}
$$

$D(R)$ is real. The number of independent elements of $D(R)$ is equal 10.

The eigenvalues and eigenvectors of $\boldsymbol{D}(R)$:

$\omega^2_{4,1}(R) = \omega^2_{4,1}(\Gamma)$ (threefold degenerate)

$$\boldsymbol{e}^T(R; 4, 1, 1) = \frac{1}{\sqrt{2}}(1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

$$\boldsymbol{e}^T(R; 4, 1, 2) = \frac{1}{\sqrt{2}}(0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)$$

$$\boldsymbol{e}^T(R; 4, 1, 3) = \frac{1}{\sqrt{2}}(0, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0\ 0, 0)$$

$\omega^2_{7,1}(R) = \omega^2_{7,1}(\Gamma)$, $\boldsymbol{e}(R; 7, 1, 1) = \boldsymbol{e}(\Gamma; 7, 1, 1,)$

$\omega^2_{8,1}(R) = \omega^2_{8,1}(\Gamma)$ (twofold degenerate),

$\boldsymbol{e}(R; 8, 1, \alpha) = \boldsymbol{e}(\Gamma; 8, 1, \alpha)$ for $\alpha = 1, 2$.

$\omega^2_{9,1}(R) = \omega^2_{9,1}(\Gamma)$ (threefold degenerate)

$\boldsymbol{e}(R; 9, 1, \alpha) = \boldsymbol{e}(\Gamma; 9, 1, \alpha)$ for $\alpha = 1, 2, 3$.

$\boldsymbol{D}_{10}(R) = \boldsymbol{D}_{10}(\Gamma)$ Each eigenvalue of $\boldsymbol{D}_{10}(R)$ is threefold degenerate.

$\boldsymbol{E}^T(R; 10, 1) = (a, 0, 0, -a, 0, 0, b, c, c, b, c, -c, b, -c, c, b, -c, -c)$

$\boldsymbol{E}^T(R; 10, 2) = (0, a, 0, 0, -a, 0, c, b, -c, c, b, c, -c, b, c, -c, b, -c)$

$\boldsymbol{E}^T(R; 10, 3) = (0, 0, a, 0, 0, -a, c, -c, b, -c, c, b, c, c, b, -c, -c, b)$

Symmetry at X

$$
D(X)=\begin{bmatrix}
A & 0 & 0 & 0 & 0 & 0 & D & F & F & -D & -F & F & -D & F & -F & D & -F & -F \\
0 & B & 0 & 0 & 0 & C & G & E & H & -G & -E & H & G & -E & H & -G & E & H \\
0 & 0 & B & 0 & C & 0 & G & H & E & G & H & -E & -G & H & -E & -G & H & E \\
0 & 0 & 0 & A & 0 & 0 & -D & -F & -F & -D & -F & F & -D & F & -F & -D & F & F \\
0 & 0 & C & 0 & B & 0 & -G & -E & -H & -G & -E & H & G & -E & H & G & -E & -H \\
0 & C & 0 & 0 & 0 & B & -G & -H & -E & G & H & -E & -G & H & -E & G & -H & -E \\
D & G & G & -D & -G & -G & J & L & L & 0 & 0 & 0 & 0 & 0 & 0 & N & R & R \\
F & E & H & -F & -E & -H & L & K & M & 0 & 0 & 0 & 0 & 0 & 0 & -R & P & S \\
F & H & E & -F & -H & -E & L & M & K & 0 & 0 & 0 & 0 & 0 & 0 & -R & S & P \\
-D & -G & G & -D & -G & G & 0 & 0 & 0 & J & L & -L & N & R & -R & 0 & 0 & 0 \\
-F & -E & H & -F & -E & H & 0 & 0 & 0 & L & K & -M & -R & P & -S & 0 & 0 & 0 \\
F & H & -E & F & H & -E & 0 & 0 & 0 & -L & -M & K & R & -S & P & 0 & 0 & 0 \\
-D & G & -G & -D & G & -G & 0 & 0 & 0 & N & -R & R & J & -L & L & 0 & 0 & 0 \\
F & -E & H & F & -E & H & 0 & 0 & 0 & R & P & -S & -L & K & -M & 0 & 0 & 0 \\
-F & H & -E & -F & H & -E & 0 & 0 & 0 & -R & -S & P & L & -M & K & 0 & 0 & 0 \\
D & -G & -G & -D & G & G & N & -R & -R & 0 & 0 & 0 & 0 & 0 & 0 & J & -L & -L \\
-F & E & H & F & -E & -H & R & P & S & 0 & 0 & 0 & 0 & 0 & 0 & -L & K & M \\
-F & H & E & F & -H & -E & R & S & P & 0 & 0 & 0 & 0 & 0 & 0 & -L & M & K
\end{bmatrix}
$$

$D(X)$ is real. The number of independent elements of $D(X)$ is equal 16.

The eigenvalues and eigenvectors of $D(X)$:

$$\omega^2_{1,\alpha}(X) = \tfrac{1}{2}\{B+C+K-M+P-S\pm([B+C+K-M+P-S]^2-$$
$$-4[(B+C)(K-M+P-S)-4(H-E)^2])^{\frac{1}{2}}\}$$

where $\alpha = 1, 2$ and plus stands for $\alpha = 1$ while minus for $x = 2$.

$$e^T(X; 1, \alpha, 1) =$$
$$= \frac{1}{2\sqrt{1+N^2(\alpha)}}(0, -1, 1, 0, 1, -1, 0, N(\alpha), -N(\alpha), 0, 0, 0, 0, 0, 0, 0, N(\alpha), -N(\alpha))$$

$$e^T(X; 1, \alpha, 2) =$$
$$= \frac{1}{2\sqrt{1+N^2(\alpha)}}(0, 1, 1, 0, 1, 1, 0, 0, 0, 0, N(\alpha), N(\alpha), 0, N(\alpha), N(\alpha), 0, 0, 0)$$

where $N(\alpha) = (\omega^2_{1,\alpha}(X)-B-C)/2(H-E)$.

Each of $\omega^2_{1,\alpha}(X)$ is twofold degenerate.

$$D_2(X) = \begin{bmatrix} B-C & 2\sqrt{2}G & 2(H+E) \\ 2\sqrt{2}G & J-N & \sqrt{2}(R+L) \\ 2(H+E) & \sqrt{2}(R+L) & K+M+P+S \end{bmatrix}$$

Each eigenvalue of $\boldsymbol{D}_2(X)$ id twofold degenerate.

$$\boldsymbol{E}^T(X;2,1) = (0,\ a,\quad a,\ 0,\ -a,\ -a,\ -b,\ c,\ c,\ 0,\quad 0,\ 0,\quad 0,\quad 0,\ 0,\ b,\ c,\ c)$$

$$\boldsymbol{E}^T(X;2,2) = (0,\ a,\ -a,\ 0,\quad a,\ -a,\quad 0,\ 0,\ 0,\ b,\ -c,\ c,\ -b,\ -c,\ c,\ 0,\ 0,\ 0)$$

$$\boldsymbol{D}_3(X) = \begin{bmatrix} A & 2D & 2\sqrt{2}F \\ 2D & J+N & \sqrt{2}(L-R) \\ 2\sqrt{2}F & \sqrt{2}(L-R) & K+M-P-S \end{bmatrix}$$

Each eigenvalue of $\boldsymbol{D}_3(X)$ is twofold degenerate.

$$\boldsymbol{E}^T(X;3,1) = (-d,\ 0,\ 0,\ d,\ 0,\ 0,\ e,\ f,\ f,\ 0,\ 0,\quad 0,\ 0,\quad 0,\ 0,\ e,\ -f,\ -f)$$

$$\boldsymbol{E}^T(X;3,2) = (\ d,\ 0,\ 0,\ d,\ 0,\ 0,\ 0,\ 0,\ 0,\ e,\ f,\ -f,\ e,\ -f,\ f,\ 0,\quad 0,\quad 0)$$

$$\omega^2_{4,1}(X) = K-M-P+S \quad \text{(twofold degenerate)}$$

$$\boldsymbol{e}^T(X;4,1,1) = \tfrac{1}{2}(0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 1,\ -1,\ 0,\ 0,\ 0,\ 0,\quad 0,\quad 0,\ 0,\ -1,\ 1)$$

$$\boldsymbol{e}^T(X;4,1,2) = \tfrac{1}{2}(0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\quad 0,\ 0,\ 1,\ 1,\ 0,\ -1,\ -1,\ 0,\quad 0,\ 0)$$

Symmetry at M

$\boldsymbol{D}(M) =$

B	O	O	O	-C	O	-E	H	G	-E	H	-G	E	H	-G	E	H	G
O	B	O	-C	O	O	H	-E	-G	H	-E	G	H	E	-G	H	E	G
O	O	A	O	O	O	F	-F	D	-F	F	D	-F	-F	-D	F	F	-D
O	-C	O	B	O	O	E	-H	-G	E	-H	G	E	H	-G	E	H	G
-C	O	O	O	B	O	-H	E	G	-H	E	-G	H	E	-G	H	E	G
O	O	O	O	O	A	-F	F	-D	F	-F	-D	-F	-F	-D	F	F	-D
-E	H	F	E	-H	-F	K	-M	-R	P	-S	L	O	O	O	O	O	O
H	-E	-F	-H	E	F	-M	K	R	-S	P	-L	O	O	O	O	O	O
G	-G	D	-G	G	-D	-R	R	J	-L	L	N	O	O	O	O	O	O
-E	H	-F	E	-H	F	P	-S	-L	K	-M	R	O	O	O	O	O	O
H	-E	F	-H	E	-F	-S	P	L	-M	K	-R	O	O	O	O	O	O
-G	G	D	G	-G	-D	L	-L	-N	R	-R	J	O	O	O	O	O	O
E	H	-F	E	H	-F	O	O	O	O	O	O	K	M	-R	P	S	L
H	E	-F	H	E	-F	O	O	O	O	O	O	M	K	-R	S	P	L
-G	-G	-D	-G	-G	-D	O	O	O	O	O	O	-R	-R	J	-L	-L	N
E	H	F	E	H	F	O	O	O	O	O	O	P	S	-L	K	M	R
H	E	F	H	E	F	O	O	O	O	O	O	S	P	-L	M	K	R
G	G	-D	G	G	-D	O	O	O	O	O	O	L	L	N	R	R	J

$\boldsymbol{D}(M)$ is real. The number of independent elements of $\boldsymbol{D}(M)$ is equal 16.

The eigenvalues and eigenvectors of $\boldsymbol{D}(M)$:

$\omega^2_{1,\alpha}(M) = \omega^2_{1,\alpha}(X)$ for $\alpha = 1,2$. Each of $\omega^2_{1,\alpha}(M)$ is twofold degenerate.

$$\boldsymbol{e}^T(M;1,\alpha,1) = \frac{1}{2\sqrt{2(1+N^2(\alpha))}}(0,\ -2,\ 0,\ 2,\ 0,\ 0,\ -N(\alpha),\ -N(\alpha),$$

$$0,\ -N(\alpha),\ -N(\alpha),\ 0,\ -N(\alpha),\ N(\alpha),\ 0,\ -N(\alpha),\ N(\alpha),\ 0)$$

$$e^T(M;1,\alpha,2)=\frac{1}{2\sqrt{2(1+N^2(\alpha))}}(2,0,0,0,-2,0,N(\alpha),N(\alpha),0,N(\alpha),$$
$$N(\alpha),0,-N(\alpha),N(\alpha),0,-N(\alpha),N(\alpha),0)$$

where $N(\alpha)$ is the same as at X.

$\boldsymbol{D}_2(M)=\boldsymbol{D}_2(X)$ Each eigenvalue of $\boldsymbol{D}_2(M)$ is twofold degenerate.

$$\boldsymbol{E}^T(M;2,1)=(a,\ 0,\ 0,\ 0,\ a,\ 0,\ -b,\ b,\ -c,\ -b,\ b,\ c,\ b,\ b,\ c,\ b,\ b,\ -c)$$
$$\boldsymbol{E}^T(M;2,2)=(0,\ a,\ 0,\ a,\ 0,\ 0,\ b,\ -b,\ c,\ b,\ -b,\ -c,\ b,\ b,\ c,\ b,\ b,\ -c)$$

$\omega^2_{3,1}(M)=\omega^2_{4,1}(X)$ (twofold degenerate)

$$e^T(M;3,1,1)=\tfrac{1}{2}(0,0,0,0,0,0,1,1,0,-1,-1,0,0,0,0,0,0,0)$$
$$e^T(M;3,1,2)=\tfrac{1}{2}(0,0,0,0,0,0,0,0,0,0,0,0,1,-1,0,-1,1,0)$$

$\boldsymbol{D}_4(M)=\boldsymbol{D}_3(X)$ Each eigenvalue of $\boldsymbol{D}_4(M)$ is twofold degenerate.

$$\boldsymbol{E}^T(M;4,1)=(0,\ 0,\ d,\ 0,\ 0,\ d,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ e,\ e,\ f,\ -e,\ -e,\ f)$$
$$\boldsymbol{E}^T(M;4,2)=(0,\ 0,\ -d,\ 0,\ 0,\ d,\ e,\ -e,\ f,\ -e,\ e,\ f,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0)$$

Symmetry along Δ

$$D(\Delta)=\left[\begin{array}{cccccccccccccccccc}
a & 0 & 0 & A & 0 & 0 & \varrho D & \varrho E & \varrho E & D^* & E^* & -E^* & D^* & -E^* & E^* & \varrho D & -\varrho E & -\varrho E \\
0 & b & 0 & 0 & B & C & \varrho F & \varrho G & \varrho H & F^* & G^* & -H^* & -F^* & G^* & -H^* & -\varrho F & \varrho G & \varrho H \\
0 & 0 & b & 0 & C & B & \varrho F & \varrho H & \varrho G & -F^* & -H^* & G^* & F^* & -H^* & G^* & -\varrho F & \varrho H & \varrho G \\
A^* & 0 & 0 & a & 0 & 0 & D^* & E^* & E^* & D & E & -E & D & -E & E & D^* & -E^* & -E^* \\
0 & B^* & C^* & 0 & b & 0 & F^* & G^* & H^* & F & G & -H & -F & G & -H & -F^* & G^* & H^* \\
0 & C^* & B^* & 0 & 0 & b & F^* & H^* & G^* & -F & -H & G & F & -H & G & -F^* & H^* & G^* \\
\varrho^*D^* & \varrho^*F^* & \varrho^*F^* & D & F & F & c & f & f & J^* & M^* & N^* & J^* & N^* & M^* & g & m & m \\
\varrho^*E^* & \varrho^*G^* & \varrho^*H^* & E & G & H & f & d & e & M^* & L^* & P^* & -N^* & R^* & -P^* & -m & h & j \\
\varrho^*E^* & \varrho^*H^* & \varrho^*G^* & E & H & G & f & e & d & -N^* & -P^* & R^* & M^* & P^* & L^* & -m & j & h \\
D & F & -F & D^* & F^* & -F^* & J & M & -N & c & f & -f & g & m & -m & J & N & -M \\
E & G & -H & E^* & G^* & -H^* & M & L & -P & f & d & -e & -m & h & -j & -N & R & P \\
-E & -H & G & -E^* & -H^* & G^* & N & P & R & -f & -e & d & m & -j & h & -M & -P & L \\
D & -F & F & D^* & -F^* & F^* & J & -N & M & g & -m & m & c & -f & f & J & -M & N \\
-E & G & -H & -E^* & G^* & -H^* & N & R & P & m & h & -j & -f & d & -e & -M & L & -P \\
E & -H & G & E^* & -H^* & G^* & M & -P & L & -m & -j & h & f & -e & d & -N & P & R \\
\varrho^*D^* & -\varrho F^* & -\varrho F^* & D & -F & -F & g & -m & -m & J^* & -N^* & -M^* & J^* & -M^* & -N^* & c & -f & -f \\
-\varrho E^* & \varrho^*G^* & \varrho^*H^* & -E & G & H & m & h & j & N^* & R^* & -P^* & -M^* & L^* & P^* & -f & d & e \\
-\varrho E^* & \varrho^*H^* & \varrho^*G^* & -E & H & G & m & j & h & -M^* & P^* & L^* & N^* & -P^* & R^* & -f & e & d
\end{array}\right]$$

The small letters stand for real elements and the capitals for complex ones. $\varrho=\exp[-i\pi\xi]$.

A,B,J,L,M,N,P,R have the argument $\varphi=-\frac{\pi}{2}\xi+n\pi$, and C has the argument $\varphi=\frac{\pi}{2}(1-\xi)+n\pi$, where $n=0$ or $n=1$.

The eigenvalues and eigenvectors of $\boldsymbol{D}(\Delta)$:

$$\boldsymbol{D}_1(\Delta) = \begin{bmatrix} a+\gamma^*A & \sqrt{2}(\gamma D+D^*) & 2(\gamma E+E^*) \\ \sqrt{2}(\gamma^*D^*+D) & c+g & \sqrt{2}[f-m \\ & +2\gamma J^* & +\gamma(M^*-N^*)] \\ 2(\gamma^*E^*+E) & \sqrt{2}[f-m & d+e-h-j \\ & +\gamma^*(M-N)] & +\gamma(L^*-R^*-2P^*) \end{bmatrix}$$

$\boldsymbol{E}^T(\Delta; 1, 1) = (\gamma a,\ 0,\ 0,\ a,\ 0,\ 0,\ b,\ c,\ c,\ \gamma b,\ \gamma c,\ -\gamma c,\ \gamma b,\ -\gamma c,\ \gamma c,\ b,\ -c,\ -c)$

$\boldsymbol{E}(\Delta; 1, 1)$ is $LA+\ldots$

$$\omega^2_{2,1}(\Delta) = d-e-h+j-\gamma(L^*-R^*+2P^*)$$

$$\boldsymbol{e}^T(\Delta; 2, 1, 1) = \frac{\gamma^{*\frac{3}{2}}}{2\sqrt{2}}(0, 0, 0, 0, 0, 0, 0, 1, -1, 0, -\gamma, -\gamma, 0, \gamma, \gamma, 0, -1, 1)$$

$$\omega^2_{3,1}(\Delta) = d-e-h+j+\gamma(L^*-R^*+2P^*)$$

$$\boldsymbol{e}^T(\Delta; 3, 1, 1) = \frac{\gamma^{*\frac{3}{2}}}{2\sqrt{2}}(0, 0, 0, 0, 0, 0, 0, 1, -1, 0, \gamma, \gamma, 0, -\gamma, -\gamma, 0, -1, 1)$$

$$\boldsymbol{D}_4(\Delta) = \begin{bmatrix} a-\gamma^*A & \sqrt{2}(\gamma D-D^*) & 2(\gamma E-E^*) \\ \sqrt{2}(\gamma^*D^*-D) & c+g & \sqrt{2}[f-m \\ & -2\gamma J^* & -\gamma(M^*-N^*)] \\ 2(\gamma^*E^*-E) & \sqrt{2}[f-m & d+e-h-j \\ & -\gamma^*(M-N)] & +\gamma(R^*-L^*+2P^*) \end{bmatrix}$$

$\boldsymbol{E}^T(\Delta; 4, 1) = (\gamma d,\ 0,\ 0,\ -d,\ 0,\ 0,\ e,\ f,\ f,\ -\gamma e,\ -\gamma f,\ \gamma f,\ -\gamma e,\ \gamma f,\ -\gamma f,\ e,\ -f,\ -f)$

$$\boldsymbol{D}_5(\Delta) = \begin{bmatrix} b-\gamma^*B & \gamma^*C & \sqrt{2}(\gamma F-F^*) & \sqrt{2}(\gamma G-G^*) & \sqrt{2}(\gamma H-H^*) \\ \gamma C^* & b+\gamma^*B & \sqrt{2}(\gamma F+F^*) & \sqrt{2}(\gamma H+H^*) & \sqrt{2}(\gamma G+G^*) \\ \sqrt{2}(\gamma^*F-F) & \sqrt{2}(\gamma^*F^*+F) & c-g & f+m & f+m \\ & & & -\gamma(M^*+N^*) & +\gamma(M^*+N^*) \\ \sqrt{2}(\gamma^*G^*-G) & \sqrt{2}(\gamma^*H^*+H) & f+m & d+h & e+j \\ & & -\gamma^*(M+N) & -\gamma(L^*+R^*) & \\ \sqrt{2}(\gamma^*H^*-H) & \sqrt{2}(\gamma^*G^*+G) & f+m & e+j & d+h \\ & & +\gamma^*(M+N) & & +\gamma(L^*+R^*) \end{bmatrix}$$

Each eigenvalue of $\boldsymbol{D}_5(\Delta)$ is twofold degenerate.

$\boldsymbol{E}^T(\Delta; 5, 1) = (0,\ \gamma g,\ \gamma h, 0, -g, h,\ j,\ k,\ l,\ -\gamma j,\ -\gamma k,\ \gamma l, \gamma j, -\gamma k,\ \gamma l,\ -j,\ k,\ l)$

$\boldsymbol{E}^T(\Delta; 5, 2) = (0, -\gamma h, -\gamma g, 0, -h, g, -j, -l, -k, -\gamma j, -\gamma l,\ \gamma k, \gamma j,\ -\gamma l,\ \gamma k,\ j, -l, -k)$

$\boldsymbol{E}(\Delta; 5, 1)$ is TA+... and $\boldsymbol{E}(\Delta; 5,2)$ is TA+...

$$\gamma = \exp\left[-i\frac{\pi}{2}\xi\right].$$

Symmetry along T

$$
D(T)=\begin{bmatrix}
a & 0 & 0 & A & C & 0 & D & H & E & D & H & -E & -\varrho D^* & \varrho H^* & -\varrho E^* & -\varrho D^* & \varrho H^* & \varrho E^* \\
0 & a & 0 & C & A & 0 & H & D & -E & H & D & E & \varrho H^* & -\varrho D^* & -\varrho E^* & \varrho H^* & -\varrho D^* & \varrho E^* \\
0 & 0 & b & 0 & 0 & B & F & -F & G & -F & F & G & -\varrho F^* & -\varrho F^* & -\varrho G^* & \varrho F^* & \varrho F^* & -\varrho G^* \\
A^* & C^* & 0 & a & 0 & 0 & -D^* & -H^* & -E^* & -D^* & -H^* & E^* & -D & H & -E & -D & H & E \\
C^* & A^* & 0 & 0 & a & 0 & -H^* & -D^* & E^* & -H^* & -D^* & -E^* & H & -D & -E & H & -D & E \\
0 & 0 & B^* & 0 & 0 & b & -F^* & F^* & -G^* & F^* & -F^* & -G^* & -F & -F & -G & F & F & -G \\
D^* & H^* & F^* & -D & -H & -F & c & e & f & g & j & m & J & P & M & K & -P & -N \\
H^* & D^* & -F^* & -H & -D & F & e & c & -f & j & g & -m & -P & K & N & P & J & -M \\
E^* & -E^* & G^* & -E & E & -G & f & -f & d & -m & m & h & M & -N & L & N & -M & L \\
D^* & H^* & -F^* & -D & -H & F & g & j & -m & c & e & -f & K & -P & N & J & P & -M \\
H^* & D^* & F^* & -H & -D & -F & j & g & m & e & c & f & P & J & M & -P & K & -N \\
-E^* & E^* & G^* & E & -E & -G & m & -m & h & -f & f & d & -N & M & L & -M & N & L \\
-\varrho^* D & \varrho^* H & -\varrho^* F & -D^* & H^* & -F^* & J^* & -P^* & M^* & K^* & P^* & -N^* & c & -e & f & g & -j & m \\
\varrho^* H & -\varrho^* D & -\varrho^* F & H^* & -D^* & -F^* & P^* & K^* & -N^* & -P^* & J^* & M^* & -e & c & f & -j & g & m \\
-\varrho^* E & -\varrho^* E & -\varrho^* G & -E^* & -E^* & -G^* & M^* & N^* & L^* & N^* & M^* & L^* & f & f & d & -m & -m & h \\
-\varrho^* D & \varrho^* H & \varrho^* F & -D^* & H^* & F^* & K^* & P^* & N^* & J^* & -P^* & -M^* & g & -j & -m & c & -e & -f \\
\varrho^* H & -\varrho^* D & \varrho^* F & H^* & -D^* & F^* & -P^* & J^* & -M^* & P^* & K^* & N^* & -j & g & -m & -e & c & -f \\
\varrho^* E & \varrho^* E & -\varrho^* G & E^* & E^* & -G^* & -N^* & -M^* & L^* & -M^* & -N^* & L^* & m & m & h & -f & -f & d
\end{bmatrix}
$$

The small letters stand for real elements and the capitals for complex ones. $\varrho = \exp[-i\pi\xi]$.

A, B, J, K, L, M, N, P have the argument $\varphi = \frac{\pi}{2}(1-\xi)+n\pi$, and C has the argument $\varphi = -\frac{\pi}{2}\xi + n\pi$, where $n=0$ or $n=1$.

The eigenvalues and eigenvectors of $\boldsymbol{D}(T)$:

$$
\boldsymbol{D}_1(T) = \begin{bmatrix}
b+\delta^*B & 2(F-\delta F^*) & \sqrt{2}(G-\delta G^*) \\
2(F^*-\delta^*F) & c-e-g+j & \sqrt{2}[f+m \\
 & -\delta^*(J-K+2P) & -\delta^*(M-N)] \\
\sqrt{2}(G^*-\delta^*G) & \sqrt{2}[f+m & d+h \\
 & -\delta(M^*-N^*)] & -2\delta^*L
\end{bmatrix}
$$

$$
\boldsymbol{E}^T(T;1,1) = (0,\ 0,\ \delta a,\ 0,\ 0,\ a,\ \delta b,\ -\delta b,\ \delta c,\ -\delta b,\ \delta b,\ \delta c,\ -b,\ -b,\ -c,\ b,\ b,\ -c)
$$

$$
\omega^2_{2,1}(T) = c+e-g-j+\delta^*(J-K-2P)
$$

$$
\boldsymbol{e}^T(T;2,1,1) = \frac{i\varrho^{*\frac{3}{4}}}{2\sqrt{2}}(0,0,0,0,0,0,\delta,\delta,0,-\delta,-\delta,0,1,-1,0,-1,1,0)
$$

$$
\omega^2_{3,1}(T) = c+e-g-j-\delta^*(J-K-2P)
$$

$$
\boldsymbol{e}^T(T;3,1,1) = \frac{i\varrho^{*\frac{3}{4}}}{2\sqrt{2}}(0,0,0,0,0,0,\delta,\delta,0,-\delta,-\delta,0,-1,1,0,1,-1,0)
$$

$$
D_4(T) = \begin{bmatrix} b-\delta^*B & 2(F+\delta F^*) & \sqrt{2}(G+\delta G^*) \\ 2(F^*+\delta^*F) & c-e-g+j & \sqrt{2}[f+m \\ & +\delta^*(J-K+2P) & +\delta^*(M-N)] \\ \sqrt{2}(G^*+\delta^*G) & \sqrt{2}[f+m & d+h \\ & +\delta(M^*-N^*)] & +2\delta^*L \end{bmatrix}
$$

$$
E^T(T;4,1) = (0,\ 0,\ \delta d,\ 0,\ 0,\ -d,\ \delta e,\ -\delta e,\ \delta f,\ -\delta e,\ \delta e,\ \delta f,\ e,\ e,\ f,\ -e,\ -e,\ f)
$$

$$
D_5(T) = \begin{bmatrix} a & \delta^*(A+C) & \sqrt{2}(D+H) & \delta\sqrt{2}(D^*-H^*) & 2\delta E^* \\ \delta(A^*+C^*) & a & -\delta\sqrt{2}(D^*+H^*) & \sqrt{2}(H-D) & -2E \\ \sqrt{2}(D^*+H^*) & -\delta^*\sqrt{2}(D+H) & c+e+g+j & \delta^*(J+K) & \delta^*\sqrt{2}(M+N) \\ \delta^*\sqrt{2}(D-H) & \sqrt{2}(H^*-D^*) & \delta(J^*+K^*) & c-e+g-j & \sqrt{2}(f-m) \\ 2\delta^*E & -2E^* & \delta\sqrt{2}(M^*+N^*) & \sqrt{2}(f-m) & d-h \end{bmatrix}
$$

Each eigenvalue of $D_5(T)$ is twofold degenerate.

$$
E^T(T;5,1) = (\delta g,\ \delta g,\ 0,\ h,\ h,\ 0,\ \delta j,\ \delta j,\ 0,\ \delta j,\ \delta j,\ 0,\ k,\ k,\ l,\ k,\ k,\ -1)
$$

$$
E^T(T;5,2) = (-\delta h,\ \delta h,\ 0,\ -g,\ g,\ 0,\ \delta k,\ -\delta k,\ \delta l,\ \delta k,\ -\delta k,\ -\delta l,\ j,\ -j,\ 0,\ j,\ -j,\ 0)
$$

$$
\delta = \exp\left[-i\frac{\pi}{2}(1+\xi)\right].
$$

Symmetry along Λ

$D(\Lambda) =$

a	b	b	A	B	B	ϱD	ϱE	ϱE	ϱG	ϱF	ϱH	ϱG	ϱH	ϱF	γJ	γL	γL
b	a	b	B	A	B	ϱF	ϱG	ϱH	ϱE	ϱD	ϱE	ϱH	ϱG	ϱF	γL	γJ	γL
b	b	a	B	B	A	ϱF	ϱH	ϱG	ϱH	ϱF	ϱG	ϱE	ϱE	ϱD	γL	γL	γJ
A^*	B^*	B^*	a	b	b	D^*	E^*	E^*	G^*	F^*	H^*	G^*	H^*	F^*	J^*	L^*	L^*
B^*	A^*	B^*	b	a	b	F^*	G^*	H^*	E^*	D^*	E^*	H^*	G^*	F^*	L^*	J^*	L^*
B^*	B^*	A^*	b	b	a	F^*	H^*	G^*	H^*	F^*	G^*	E^*	E^*	D^*	L^*	L^*	J^*
ϱ^*D^*	ϱ^*F^*	ϱ^*F^*	D	F	F	c	e	e	j	n	p	j	p	n	M	P	P
ϱ^*E^*	ϱ^*G^*	ϱ^*H^*	E	G	H	e	d	f	m	j	r'	r	k	p	R	N	S
ϱ^*E^*	ϱ^*H^*	ϱ^*G^*	E	H	G	e	f	d	r	p	k	m	r	j	R	S	N
ϱ^*G^*	ϱ^*E^*	ϱ^*H^*	G	E	H	j	m	r	d	e	f	k	r	p	N	R	S
ϱ^*F^*	ϱ^*D^*	ϱ^*F^*	F	D	F	n	j	p	e	c	e	p	j	n	P	M	P
ϱ^*H^*	ϱ^*E^*	ϱ^*G^*	H	E	G	p	r	k	f	e	d	r	m	j	S	R	N
ϱ^*G^*	ϱ^*H^*	ϱ^*E^*	G	H	E	j	r	m	k	p	r	d	f	e	N	S	R
ϱ^*H^*	ϱ^*G^*	ϱ^*E^*	H	G	E	p	k	r	r	j	m	f	d	e	S	N	R
ϱ^*F^*	ϱ^*F^*	ϱ^*D^*	F	F	D	n	p	j	p	n	j	e	e	c	P	P	M
γ^*J^*	γ^*L^*	γ^*L^*	J	L	L	M^*	R^*	R^*	N^*	P^*	S^*	N^*	S^*	P^*	g	h	h
γ^*L^*	γ^*J^*	γ^*L^*	L	J	L	P^*	N^*	S^*	R^*	M^*	R^*	S^*	N^*	P^*	h	g	h
γ^*L^*	γ^*L^*	γ^*J^*	L	L	J	P^*	S^*	N^*	S^*	P^*	N^*	R^*	R^*	M^*	h	h	g

The small letters stand for real elements and the capitals for complex ones. $\varrho = \exp[-i\pi\xi]$ and $\gamma = \varrho^3$.

M,N,P,R,S have the argument $\varphi = -\pi\xi + n\pi$, where $n=0$ or $n=1$.

The eigenvalues and eigenvectors of $\boldsymbol{D}(\Lambda)$:

$$\boldsymbol{D}_1(\Lambda)=\begin{bmatrix} a+2b & A+2B & \varrho(D+2F) & \varrho\sqrt{2}(E+G+H) & \gamma(J+2L) \\ A^*+2B^* & a+2b & D^*+2F^* & \sqrt{2}(E^*+G^*+H^*) & J^*+2L^* \\ \varrho^*(D^*+2F^*) & D+2F & c+2n & \sqrt{2}(e+j+p) & M+2P \\ \varrho^*\sqrt{2}(E^*+G^*+H^*) & \sqrt{2}(E+G+H) & \sqrt{2}(e+j+p) & d+f+k+m+2r & \sqrt{2}(R+N+S) \\ \gamma^*(J^*+2L^*) & J+2L & M^*+2P^* & \sqrt{2}(R^*+N^*+S^*) & g+2h \end{bmatrix}$$

$\boldsymbol{E}^T(\Lambda;1,1)=(a,\ a,\ a,\ b,\ b,\ b,\ c,\ d,\ d,\ d,\ c,\ d,\ d,\ d,\ c,\ e,\ e,\ e)$

$\boldsymbol{E}(\Lambda;1,1)$ is LA+...

$\omega^3_{2,1}(\Lambda)=d-f-k-m+2r$

$$\boldsymbol{e}^T(\Lambda;2,1,1)=\frac{\varrho^{*5/4}}{\sqrt{6}}(0,0,0,0,0,0,0,1,-1,-1,0,1,1,-1,0,0,0,0)$$

$$\boldsymbol{D}_3(\Lambda)=\begin{bmatrix} a-b & A-B & \varrho(D-F) & \frac{\varrho}{\sqrt{2}}(2G-E-H) & \frac{\varrho}{\sqrt{2}}(2H-E-G) & \gamma(J-L) \\ A^*-B^* & a-b & D^*-F^* & \frac{1}{\sqrt{2}}(2G^*-E^*-H^*) & \frac{1}{\sqrt{2}}(2H^*-E^*-G^*) & J^*-L^* \\ \varrho^*(D^*-F^*) & D-F & c-n & \frac{1}{\sqrt{2}}(2j-e-p) & \frac{1}{\sqrt{2}}(2p-e-j) & M-P \\ \frac{\varrho^*}{\sqrt{2}}(2G^*-E^*-H^*) & \frac{1}{\sqrt{2}}(2G-E-H) & \frac{1}{\sqrt{2}}(2j-e-p) & d+k-r-\frac{1}{2}(m+f) & f-\frac{1}{2}(d+k+m-r) & \frac{1}{\sqrt{2}}(2N-R-S) \\ \frac{\varrho^*}{\sqrt{2}}(2H^*-E^*-G^*) & \frac{1}{\sqrt{2}}(2H-E-G) & \frac{1}{\sqrt{2}}(2p-e-j) & f-\frac{1}{2}(d+k+m-r) & d+m-r-\frac{1}{2}(k+f) & \frac{1}{\sqrt{2}}(2S-N-R) \\ \gamma^*(J^*-L^*) & J-L & M^*-P^* & \frac{1}{\sqrt{2}}(2N^*-R^*-S^*) & \frac{1}{\sqrt{2}}(2S^*-N^*-R^*) & g-h \end{bmatrix}$$

Each eigenvalue of $\boldsymbol{D}_3(\Lambda)$ is twofold degenerate.

$\boldsymbol{E}^T(\Lambda; 3, 1) =$

$(a,\ a,\ -2a,\ b,\ b,\ -2b,\ c,\ d-2e,\ e-2d,\ d-2e,\ c,\ e-2d,\ d+e,\ d+e,\ -2c,\ f,\ f,\ -2f)$

$\boldsymbol{E}^T(\Lambda; 3, 2) = \sqrt{3}(-a,\ a,\ 0,\ -b,\ b,\ 0,\ -c,\ d,\ e,\ -d,\ c,\ -e,\ e-d,\ d-e,\ 0,\ -f,\ f,\ 0)$

$\boldsymbol{E}(\Lambda; 3, 1)$ is TA+... and $\boldsymbol{E}(\Lambda; 3, 2)$ is TA+...

Symmetry along Σ

$$
\boldsymbol{D}(\Sigma) = \begin{bmatrix}
a & c & A & B & D & E & \varrho F & \varrho G & \varrho H & \varrho F^* & \varrho G^* & -\varrho H^* & K & M & N & \gamma K^* & \gamma M^* & -\gamma N^* \\
c & a & A & D & B & E & \varrho G^* & \varrho F^* & -\varrho H^* & \varrho G & \varrho F & \varrho H & M & K & N & \gamma M^* & \gamma K^* & -\gamma N^* \\
A^* & A^* & b & E & E & C & \varrho J & -\varrho J^* & \varrho u & -\varrho J^* & \varrho J & \varrho u & P & P & L & -\gamma P^* & -\gamma P^* & \gamma L^* \\
B^* & D^* & E^* & a & c & -A & F^* & G^* & H^* & F & G & -H & K^* & M^* & N^* & K & M & -N \\
D^* & B^* & E^* & c & a & -A & G & F & -H & G^* & F^* & H^* & M^* & K^* & N^* & M & K & -N \\
E^* & E^* & C^* & -A^* & -A^* & b & J^* & -J & u & -J & J^* & u & P^* & P^* & L^* & -P & -P & L \\
\varrho^* F^* & \varrho^* G & \varrho^* J^* & F & G^* & J & d & f & g & p & s & t & R^* & S^* & T^* & W & U & -V \\
\varrho^* G^* & \varrho^* F & -\varrho^* J & G & F^* & -J^* & f & d & -g & s & p & -t & U^* & W^* & V^* & S & R & -T \\
\varrho^* H^* & -\varrho^* H & \varrho^* u & H & -H^* & u & g & -g & e & -t & t & r & X^* & Y^* & Z^* & -Y & -X & Z \\
\varrho^* F & \varrho^* G^* & -\varrho^* J & F^* & G & -J^* & p & s & -t & d & f & -g & W^* & U^* & V^* & R & S & -T \\
\varrho^* G & \varrho^* F^* & \varrho^* J^* & G^* & F & J & s & p & t & f & d & g & S^* & R^* & T^* & U & W & -V \\
-\varrho^* H & \varrho^* H^* & \varrho^* u & -H^* & H & u & t & -t & r & -g & g & e & Y^* & X^* & Z^* & -X & -Y & Z \\
K^* & M^* & P^* & K & M & P & R & U & X & W & S & Y & h & m & n & I & \Delta & \Sigma \\
M^* & K^* & P^* & M & K & P & S & W & Y & U & R & X & m & h & n & \Delta & I & \Sigma \\
N^* & N^* & L^* & N & N & L & T & V & Z & V & T & Z & n & n & j & -\Sigma & -\Sigma & \Lambda \\
\gamma^* K & \gamma^* M & -\gamma^* P & K^* & M^* & -P^* & W^* & S^* & -Y^* & R^* & U^* & -X^* & I^* & \Delta^* & -\Sigma^* & h & m & -n \\
\gamma^* M & \gamma^* K & -\gamma^* P & M^* & K^* & -P^* & U^* & R^* & -X^* & S^* & W^* & -Y^* & \Delta^* & I^* & -\Sigma^* & m & h & -n \\
-\gamma^* N & -\gamma^* N & \gamma^* L & -N^* & -N^* & L^* & -V^* & -T^* & Z^* & -T^* & -V^* & Z^* & \Sigma^* & \Sigma^* & \Lambda^* & -n & -n & j
\end{bmatrix}
$$

The small letters stand for real elements and the capitals for complex ones. $\varrho = \exp[-i\pi\xi]$ and $\gamma = \varrho^2$.
A has the argument $\varphi = \frac{\pi}{2} + n\pi$, B,C,D,I,Δ,Σ,Λ have the argument $\varphi = -\pi\xi + n\pi$, R,S,T,U,W,V,X,Y,Z have the argument $\varphi = -\frac{\pi}{2}\xi + n\pi$, and E has the argument $\varphi = \pi\left(\frac{1}{2} - \xi\right) + n\pi$, where $n = 0$ or $n = 1$.

The eigenvalues and eigenvectors of $\boldsymbol{D}(\Sigma)$:

$$
\boldsymbol{D}_1(\Sigma) = \begin{bmatrix}
a+c+\varrho^*(B+D) & \sqrt{2}(A-\varrho^* E) & F+G+F^*+G^* & K+M+\varrho(K^*+M^*) & \sqrt{2}(N+\varrho N^*) \\
\sqrt{2}(A^*-\varrho E^*) & b-\varrho^* C & \sqrt{2}(J-J^*) & \sqrt{2}(P-\varrho P^*) & L-\varrho L^* \\
F^*+G^*+F+G & \sqrt{2}(J^*-J) & d+f+p+s & R+S+U+W & \sqrt{2}(T+V) \\
K^*+M^*+\varrho^*(K+M) & \sqrt{2}(P^*-\varrho^* P) & R^*+S^*+U^*+W^* & h+m+\varrho^*(I+\Delta) & \sqrt{2}(n-\varrho^*\Sigma) \\
\sqrt{2}(N^*+\varrho^* N) & L^*-\varrho^* L & \sqrt{2}(T^*+V^*) & \sqrt{2}(n-\varrho\Sigma^*) & j-\varrho^*\Lambda
\end{bmatrix}
$$

$$\boldsymbol{E}^T(\Sigma; 1, 1) = (\varrho a,\ \varrho a,\ \varrho b,\ a,\ a,\ -b,\ c,\ c,\ 0,\ c,\ c,\ 0,\ \varrho d,\ \varrho d,\ \varrho e,\ d,\ d,\ -e)$$

$\boldsymbol{E}(\Sigma; 1, 1)$ is LA+...

$$\boldsymbol{D}_2(\Sigma) = \begin{bmatrix} a-c & F+G & K-M \\ -\varrho^*(B-D) & -F^*-G^* & -\varrho(K^*-M^*) \\ F^*+G^* & d+f & R-S \\ -F-G & -p-s & +U-W \\ K^*-M^* & R^*-S^* & h-m \\ -\varrho^*(K-M) & +U^*-W^* & -\varrho^*(I-\Delta) \end{bmatrix}$$

$$\boldsymbol{E}^T(\Sigma; 2, 1) = (\varrho f,\ -\varrho f,\ 0,\ -f,\ f,\ 0,\ g,\ g,\ 0,\ -g,\ -g,\ 0,\ \varrho h,\ -\varrho h,\ 0,\ -h,\ h,\ 0)$$

$$\boldsymbol{D}_3(\Sigma) = \begin{bmatrix} a-c & F-G & \sqrt{2}(H+H^*) & K-M \\ +\varrho^*(B-D) & +F^*-G^* & & +\varrho(K^*-M^*) \\ F^*-G^* & d-f & \sqrt{2}(g-t) & R-S \\ +F-G & +p-s & & -U+W \\ \sqrt{2}(H^*+H) & \sqrt{2}(g-t) & e-r & \sqrt{2}(X-Y) \\ K^*-M^* & R^*-S^* & \sqrt{2}(X^*-Y^*) & h-m \\ +\varrho^*(K-M) & -U^*+W^* & & +\varrho^*(I-\Delta) \end{bmatrix}$$

$$\boldsymbol{E}^T(\Sigma; 3, 1) = (\varrho j,\ -\varrho j,\ 0,\ j,\ -j,\ 0,\ k,\ -k,\ l,\ k,\ -k,\ -l,\ \varrho m,\ -\varrho m,\ 0,\ m,\ -m,\ 0)$$

$\boldsymbol{E}(\Sigma; 3, 1)$ is TA+...

$\boldsymbol{D}_4(\Sigma) =$

$$= \begin{bmatrix} a+c & \sqrt{2}(A+\varrho^*E) & F-G & \sqrt{2}(H-H^*) & K+M & \sqrt{2}(N-\varrho N^*) \\ -\varrho^*(B+D) & & -F^*+G^* & & -\varrho(K^*+M^*) & \\ \sqrt{2}(A^*+\varrho E^*) & b+\varrho^*C & \sqrt{2}(J+J^*) & 2u & \sqrt{2}(P+\varrho P^*) & L+\varrho L^*) \\ F^*-G^* & \sqrt{2}(J^*+J) & d-f & \sqrt{2}(g+t) & R+S & \sqrt{2}(T-V) \\ -F+G & & -p+s & & -U-W & \\ \sqrt{2}(H^*-H) & 2u & \sqrt{2}(g+t) & e+r & \sqrt{2}(X+Y) & 2Z \\ K^*+M^* & \sqrt{2}(P^*+\varrho^*P) & R^*+S^* & \sqrt{2}(X^*+Y^*) & h+m & \sqrt{2}(n+\varrho^*\Sigma) \\ -\varrho^*(K+M) & & -U^*-W^* & & -\varrho^*(I+\Delta) & \\ \sqrt{2}(N^*-\varrho^*N) & L^*+\varrho^*L & \sqrt{2}(T^*-V^*) & 2Z^* & \sqrt{2}(n+\varrho\Sigma^*) & j+\varrho^*\Lambda \end{bmatrix}$$

$$\boldsymbol{E}^T(\Sigma; 4, 1) = (\varrho n,\ \varrho n,\ \varrho p,\ -n,\ -n,\ p,\ r,\ -r,\ s,\ -r,\ r,\ s,\ \varrho t,\ \varrho t,\ \varrho u,\ -t,\ -t,\ u)$$

$\boldsymbol{E}(\Sigma; 4, 1)$ is TA+...

Symmetry along S

$$
D(S)=\left[\begin{array}{cccccccccccccccccc}
a & A & A & B & E & E & F & J & J & \varrho u & \varrho N & -\varrho N^* & \varrho u & -\varrho N^* & \varrho N & \gamma F^* & -\gamma J^* & -\gamma J^* \\
A^* & b & c & E & C & D & K & G & H & \varrho P & \varrho L & \varrho M & -\varrho P^* & \varrho L^* & \varrho M^* & -\gamma K^* & \gamma G^* & \gamma H^* \\
A^* & c & b & E & D & C & K & H & G & -\varrho P^* & \varrho M^* & \varrho L^* & \varrho P & \varrho M & \varrho L & -\gamma K^* & \gamma H^* & \gamma G^* \\
B^* & E^* & E^* & a & -A & -A & -F^* & -J^* & -J^* & u & N^* & -N & u & -N & N^* & -F & J & J \\
E^* & C^* & D^* & -A^* & b & c & -K^* & -G^* & -H^* & P^* & L^* & M^* & -P & L & M & K & -G & -H \\
E^* & D^* & C^* & -A^* & c & b & -K^* & -H^* & -G^* & -P & M & L & P^* & M^* & L^* & K & -H & -G \\
F^* & K^* & K^* & -F & -K & -K & d & g & g & R & S & T & R & T & S & I & \Delta & \Delta \\
J^* & G^* & H^* & -J & -G & -H & g & e & f & U & W & V & X & Z & Y & -\Delta & \Lambda & \Sigma \\
J^* & H^* & G^* & -J & -H & -G & g & f & e & X & Y & Z & U & V & W & -\Delta & \Sigma & \Lambda \\
\varrho^* u & \varrho^* P^* & -\varrho^* P & u & P & -P^* & R^* & U^* & X^* & h & n & -n & p & -t & t & R & -X & -U \\
\varrho^* N^* & \varrho^* L^* & \varrho^* M & N & L & M^* & S^* & W^* & Y^* & n & j & m & t & r & s & -T & Z & V \\
-\varrho^* N & \varrho^* M^* & \varrho^* L & -N^* & M & L^* & T^* & V^* & Z^* & -n & m & j & -t & s & r & -S & Y & W \\
\varrho^* u & -\varrho^* P & \varrho^* P^* & u & -P^* & P & R^* & X^* & U^* & p & t & -t & h & -n & n & R & -U & -X \\
-\varrho^* N & \varrho^* L & \varrho^* M^* & -N^* & L^* & M & T^* & Z^* & V^* & -t & r & s & -n & j & m & -S & W & Y \\
\varrho^* N^* & \varrho^* M & \varrho^* L^* & N & M^* & L & S^* & Y^* & W^* & t & s & r & n & m & j & -T & V & Z \\
\gamma^* F & -\gamma^* K & -\gamma^* K & -F^* & K^* & K^* & I^* & -\Delta^* & -\Delta^* & R^* & -T^* & -S^* & R^* & -S^* & -T^* & d & -g & -g \\
-\gamma^* J & \gamma^* G & \gamma^* H & J^* & -G^* & -H^* & \Delta^* & \Lambda^* & \Sigma^* & -X^* & Z^* & Y^* & -U^* & W^* & V^* & -g & e & f \\
-\gamma^* J & \gamma^* H & \gamma^* G & J^* & -H^* & -G^* & \Delta^* & \Sigma^* & \Lambda^* & -U^* & V^* & W^* & -X^* & Y^* & Z^* & -g & f & e
\end{array}\right]
$$

The small letters stand for real elements and the capitals for complex ones. $\varrho = \exp[-i\pi\xi]$ and $\gamma = \varrho^2$

A has the argument $\varphi = \frac{\pi}{2} + n\pi$, B,C,D,I,$\Delta$,$\Sigma$,$\Lambda$ have the argument $\varphi = -\pi\xi + n\pi$, R,S,T,U,W,V,X,Y,Z have the argument $\varphi = \frac{\pi}{2}(1-\xi) + n\pi$, and E has the argument $\varphi = \pi\left(\frac{1}{2} - \xi\right) + n\pi$, where $n = 0$ or $n = 1$.

The eigenvalues and eigenvectors of $\boldsymbol{D}(S)$:

$$
\boldsymbol{D}_1(S) = \begin{bmatrix}
a-\varrho^*B & \sqrt{2}(A+\varrho^*E) & F+\varrho F^* & \sqrt{2}(J+\varrho J^*) & \sqrt{2}(N-N^*) \\
\sqrt{2}(A^*+\varrho E^*) & b+c+\varrho^*(C+D) & \sqrt{2}(K-\varrho K^*) & G+H-\varrho(G^*+H^*) & L+M+L^*+M^* \\
F^*+\varrho^*F & \sqrt{2}(K^*-\varrho^*K) & d+\varrho^*I & \sqrt{2}(g-\varrho^*\Delta) & \varrho^*\sqrt{2}(S+T) \\
\sqrt{2}(J^*+\varrho^*J) & G^*+H^*-\varrho^*(G+H) & \sqrt{2}(g-\varrho\Delta^*) & e+f-\varrho^*(\Lambda+\Sigma) & \varrho^*(W+V+Y+Z) \\
\sqrt{2}(N^*-N) & L^*+M^*+L+M & \varrho\sqrt{2}(S^*+T^*) & \varrho(W^*+V^*+Y^*+Z^*) & j+m+r+s
\end{bmatrix}
$$

$$
\boldsymbol{E}^T(S;1,1) = (\varrho a,\ \varrho b,\ \varrho b,\ -a,\ b,\ b,\ \varrho c,\ \varrho d,\ \varrho d,\ 0,\ e,\ e,\ 0,\ e,\ e,\ c,\ -d,\ -d)
$$

$$
\boldsymbol{D}_2(S) = \begin{bmatrix}
a+\varrho^*B & \sqrt{2}(A-\varrho^*E) & F-\varrho F^* & \sqrt{2}(J-\varrho J^*) & 2u & \sqrt{2}(N+N^*) \\
\sqrt{2}(A^*-\varrho E^*) & b+c-\varrho^*(C+D) & \sqrt{2}(K+\varrho K^*) & G+H+\varrho(G^*+H^*) & \sqrt{2}(P-P^*) & L-M-L^*+M^* \\
F^*-\varrho^*F & \sqrt{2}(K^*+\varrho^*K) & d-\varrho^*I & \sqrt{2}(g+\varrho^*\Delta) & 2\varrho^*R & \varrho^*\sqrt{2}(S-T) \\
\sqrt{2}(J^*-\varrho^*J) & G^*+H^*+\varrho^*(G+H) & \sqrt{2}(g+\varrho\Delta^*) & e+f+\varrho^*(\Lambda+\Sigma) & \varrho^*\sqrt{2}(U+X) & \varrho^*(W-V+Y-Z) \\
2u & \sqrt{2}(P^*-P) & 2\varrho R^* & \varrho\sqrt{2}(U^*+X^*) & h+p & \sqrt{2}(n+t) \\
\sqrt{2}(N^*+N) & L^*-M^*-L+M & \varrho\sqrt{2}(S^*-T^*) & \varrho(W^*-V^*+Y^*-Z^*) & \sqrt{2}(n+t) & j-m-r+s
\end{bmatrix}
$$

$$E^T(S;2,1) = (\varrho f,\ \varrho g,\ \varrho g,\ f,\ -g,\ -g,\ \varrho h,\ \varrho j,\ \varrho j,\ k,\ l,\ -l,\ k,\ -l,\ l,\ -h,\ j,\ j)$$

$$D_3(S) = \begin{bmatrix} b-c & G-H & \sqrt{2}(P+P^*) & L-M \\ +\varrho^*(C-D) & -\varrho(G^*-H^*) & & +L^*-M^* \\ G^*-H^* & e-f & \varrho^*\sqrt{2}(U-X) & \varrho^*(W-V \\ -\varrho^*(G-H) & +\varrho^*(\Sigma-\Lambda) & & -Y+Z) \\ \sqrt{2}(P^*+P) & \varrho\sqrt{2}(U^*-X^*) & h-p & \sqrt{2}(n-t) \\ L^*-M^* & \varrho(W^*-V^* & \sqrt{2}(n-t) & j-m \\ +L-M & -Y^*+Z^*) & & +r-s \end{bmatrix}$$

$$E^T(S;3,1) = (0,\ \varrho m,\ -\varrho m,\ 0,\ m,\ -m,\ 0,\ \varrho n,\ -\varrho n,\ p,\ r,\ -r,\ -p,\ r,\ -r,\ 0,\ -n,\ n)$$

$$D_4(S) = \begin{bmatrix} b-c & G+H & L+M \\ +\varrho^*(D-C) & +\varrho(G^*-H^*) & -L^*-M^* \\ G^*-H^* & e-f & \varrho^*(W+V \\ +\varrho^*(G-H) & +\varrho^*(\Lambda-\Sigma) & -Y-Z \\ L^*+M^* & \varrho(W^*+V^* & j+m \\ -L-M & -Y^*-Z^*) & -r-s \end{bmatrix}$$

$$E^T(S;4,1) = (0,\ \varrho s,\ -\varrho s,\ 0,\ -s,\ s,\ 0,\ \varrho t,\ -\varrho t,\ 0,\ u,\ u,\ 0,\ -u,\ -u,\ 0,\ t,\ -t).$$

Symmetry along Z

$$D(Z)= \begin{bmatrix}
a & 0 & A & 0 & B & 0 & D & E & F & -\varrho D^* & -\varrho E^* & \varrho F^* & -D & E & -F & \varrho D^* & -\varrho E^* & -\varrho F^* \\
0 & b & 0 & B & 0 & C & G & H & J & -\varrho G^* & -\varrho H^* & \varrho J^* & G & -H & J & -\varrho G^* & \varrho H^* & \varrho J^* \\
A^* & 0 & c & 0 & C & 0 & K & L & M & \varrho K^* & \varrho L^* & -\varrho M^* & -K & L & -M & -\varrho K^* & \varrho L^* & \varrho M^* \\
0 & B^* & 0 & a & 0 & -A & -D^* & -E^* & -F^* & -D & -E & F & -D^* & E^* & -F^* & -D & E & F \\
B^* & 0 & C^* & 0 & b & 0 & -G^* & -H^* & -J^* & -G & -H & J & G^* & -H^* & J^* & G & -H & -J \\
0 & C^* & 0 & -A^* & 0 & c & -K^* & -L^* & -M^* & K & L & -M & -K^* & L^* & -M^* & K & -L & -M \\
D^* & G^* & K^* & -D & -G & -K & d & g & h & N & P & S & 0 & V & W & I & \Lambda & \Sigma \\
E^* & H^* & L^* & -E & -H & -L & g & e & j & P & R & T & V & 0 & X & -\Lambda & Y & \Delta \\
F^* & J^* & M^* & -F & -J & -M & h & j & f & -S & -T & U & -W & X & 0 & -\Sigma & \Delta & Z \\
-\varrho^* D & -\varrho^* G & \varrho^* K & -D^* & -G^* & K^* & N^* & P^* & -S^* & d & g & -h & I^* & \Lambda^* & -\Sigma^* & 0 & -V & W \\
-\varrho^* E & -\varrho^* H & \varrho^* L & -E^* & -H^* & L^* & P^* & R^* & -T^* & g & e & -j & -\Lambda^* & Y^* & -\Delta^* & -V & 0 & X \\
\varrho^* F & \varrho^* J & -\varrho^* M & F^* & J^* & -M^* & S^* & T^* & U^* & -h & -j & f & \Sigma^* & -\Delta^* & Z^* & -W & X & 0 \\
-D^* & G^* & -K^* & -D & G & -K & 0 & V^* & -W^* & I & -\Lambda & \Sigma & d & -g & h & N & -P & S \\
E^* & -H^* & L^* & E & -H & L & V^* & 0 & X^* & \Lambda & Y & -\Delta & -g & e & -j & -P & R & -T \\
-F^* & J^* & -M^* & -F & J & -M & W^* & X^* & 0 & -\Sigma & -\Delta & Z & h & -j & f & -S & T & U \\
\varrho^* D & -\varrho^* G & -\varrho^* K & -D^* & G^* & K^* & I^* & -\Lambda^* & -\Sigma^* & 0 & -V^* & -W^* & N^* & -P^* & -S^* & d & -g & -h \\
-\varrho^* E & \varrho^* H & \varrho^* L & E^* & -H^* & -L^* & \Lambda^* & Y^* & \Delta^* & -V^* & 0 & X^* & -P^* & R^* & T^* & -g & e & j \\
-\varrho^* F & \varrho^* J & \varrho^* M & F^* & -J^* & -M^* & \Sigma^* & \Delta^* & Z^* & W^* & X^* & 0 & S^* & -T^* & U^* & -h & j & f
\end{bmatrix}$$

The small letters stand for real elements and capitals for complex ones. $\varrho = \exp[-i\pi\xi]$.

A,W,V,X have the argument $\varphi = \frac{\pi}{2} + n\pi$, B,N,P,R,S,T,U have the argument $\varphi = \frac{\pi}{2}(1-\xi) + n\pi$, and C,I,Y,Z,$\Delta$,$\Sigma$,$\Lambda$ have the argument $\varphi = -\frac{\pi}{2}\xi + n\pi$, where $n=0$ or $n=1$.

The eigenvalues and eigenvectors of $D(Z)$

$$D_1(Z)=\begin{bmatrix} a & A & B & \sqrt{2}D & \sqrt{2}E & -\sqrt{2}F & \varrho\sqrt{2}D^* & -\varrho\sqrt{2}E^* & \varrho\sqrt{2}F^* \\ A^* & c & C & \sqrt{2}K & \sqrt{2}L & -\sqrt{2}M & -\varrho\sqrt{2}K^* & \varrho\sqrt{2}L^* & -\varrho\sqrt{2}M^* \\ B^* & C^* & b & -\sqrt{2}G^* & -\sqrt{2}H^* & \sqrt{2}J^* & \sqrt{2}G & -\sqrt{2}H & \sqrt{2}J \\ \sqrt{2}D^* & \sqrt{2}K^* & -\sqrt{2}G & d & V+g & W-h & I-N & P+\Lambda & S-\Sigma \\ \sqrt{2}E^* & \sqrt{2}L^* & -\sqrt{2}H & V^*+g & e & X-j & -P-\Lambda & Y+R & T-\Delta \\ -\sqrt{2}F^* & -\sqrt{2}M^* & \sqrt{2}J & W^*-h & X^*-j & f & \Sigma-S & T-\Delta & Z-U \\ \varrho^*\sqrt{2}D & -\varrho^*\sqrt{2}K & \sqrt{2}G^* & I^*-N^* & -P^*-\Lambda^* & \Sigma^*-S^* & d & V-g & W+h \\ -\varrho^*\sqrt{2}E & \varrho^*\sqrt{2}L & -\sqrt{2}H^* & P^*+\Lambda^* & Y^*+R^* & T^*-\Delta^* & V^*-g & e & -X-j \\ \varrho^*\sqrt{2}F & -\varrho^*\sqrt{2}M & \sqrt{2}J^* & S^*-\Sigma^* & T^*-\Delta^* & Z^*-U^* & W^*+h & -X^*-j & f \end{bmatrix}$$

Each eigenvalue of $D_1(Z)$ is twofold degenerate.

$$E^T(Z;1,1) = (a,\ b,\ c,\ \gamma^*a,\ -\gamma^*b,\ -\gamma^*c,\ d,\ e,\ f,\ g,\ h,\ j,\ \gamma g,\ -\gamma h,\ -\gamma j,\ -\gamma^*d,\ \gamma^*e,\ \gamma^*f)$$

$$E^T(Z;1,2) = i(-a, b, -c, \gamma^*a, \gamma^*b, -\gamma^*c, \gamma g, \gamma h, -\gamma j, -\gamma^*d, -\gamma^*e, \gamma^*f, d, -e, f, g, -h, j)$$

where $\gamma = \exp\left[-i\,\dfrac{\pi}{2}\,\xi\right]$.

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