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Symmetry Adapted Harmonic Oscillator Functions

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Quantum mechanical excited energy states of two- or three-dimensional harmonic oscillators are highly degenerate. A general method is presented to calculate the symmetry adapted quantum mechanical oscillator functions with respect to the symmetry group of the oscillator. In the special case of the tetrahedral symmetry group the method is demonstrated by detailed formulas for the two- and three-dimensional case. A computer program is also available. The method can easily be modified for other symmetry groups.

I. GENERAL DESCRIPTION

1. *Introduction*

Internal vibrations of molecules and phonons in crystals are typical systems which are described by one-, two-, and three-dimensional harmonic oscillators. Here we consider those sytems invariant under the symmetry transformations of the three-dimensional local space which belong to a certain finite symmetry group G. The coordinates of the vibrations, whose number is equal to the number of the degrees of freedom of the vibrations, can then be transformed into normal coordinates q which transform as the basis functions of the irreducible representations of G. Harmonic oscillators, whose normal coordinates transform as two- and three-dimensional irreducible representations of G, have quantum mechanical excited energies which are highly degenerate. It is therefore the purpose of this paper to present a numerical procedure to calculate the symmetry adapted quantum mechanical wave functions in the excited states. This is of considerable importance for problems involving electron-phonon coupling or a Jahn–Teller effect in solid state and molecular physics [1]. We concentrate here on two- or three-dimensional harmonic oscillators. The method can, however, easily be modified for oscillators of higher dimension, whereas the one-dimensional case is trivial.

We use the usual notation in the occupation number representation of quantum mechanics [2]. $\Psi_n(q)$ are the one-dimensional harmonic oscillator eigenfunctions belonging to the nth excited energy level $n = 0, 1, 2\ldots$.

In case of a two-dimensional or E-mode we define

$$|mn\rangle_N = \Psi_m(q_u)\, \Psi_n(q_v) \qquad \text{with} \quad m + n = N, \tag{1}$$

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where q_u, q_v are normal coordinates transforming as u and v of the irreducible representation E of G and $0 \leqslant m, n, N$ are integers. The degeneracy of the excited state of N phonons is $L_N^E = N + 1$.

In case of a three-dimensional or T-mode we define

$$|lmn\rangle_N = \Psi_l(q_1)\,\Psi_m(q_2)\,\Psi_n(q_3) \qquad \text{with} \quad l + m + n = N, \tag{2}$$

where q_1, q_2, q_3 are normal coordinates transforming as the three basis functions of the irreducible representation T and $0 \leqslant l, m, n, N$ are integers. The degeneracy in the excited state of N phonons is $L_N^T = \frac{1}{2}(N+1)(N+2)$.

The problem discussed here is to find linear combinations of $|mn\rangle_N$ with fixed N which transform as the basis functions of the irreducible representations of the symmetry group G. The method is also applied to find the linear combinations of $|lmn\rangle_N$ for N fixed.

2. *Properties of the Oscillator Functions*

For simplicity we here give only those properties, which are needed to understand the method described below. The ground state wave functions $|00\rangle_N$ and $|000\rangle_N$ are invariant under all transformations of the symmetry group G. The transformation properties of the excited state functions are conveniently described by creation and annihilation operators which are defined in the usual way [2] (A^+ denotes the Hermitian conjugate of A). In case of an E-mode

$$\begin{aligned} A^+\,|mn\rangle_N &= (m+1)^{1/2}\,|m+1n\rangle_{N+1}, \\ A\,|mn\rangle_N &= m^{1/2}\,|m-1n\rangle_{N-1}, \\ B^+\,|mn\rangle_N &= (n+1)^{1/2}\,|mn+1\rangle_{N+1}, \\ B\,|mn\rangle_N &= n^{1/2}\,|mn-1\rangle_{N-1}, \end{aligned} \tag{3}$$

or in case of a T-mode

$$\begin{aligned} A^+\,|lmn\rangle_N &= (l+1)^{1/2}\,|l+1mn\rangle_{N+1}, \\ A\,|lmn\rangle_N &= l^{1/2}\,|l-1mn\rangle_{N-1}, \\ B^+\,|lmn\rangle_N &= (m+1)^{1/2}\,|lm+1n\rangle_{N+1}, \\ B\,|lmn\rangle_N &= m^{1/2}\,|lm-1n\rangle_{N-1}, \\ C^+\,|lmn\rangle_N &= (n+1)^{1/2}\,|lmn+1\rangle_{N+1}, \\ C\,|lmn\rangle_N &= n^{1/2}\,|lmn-1\rangle_{N-1}. \end{aligned} \tag{4}$$

The creation and annihilation operators are linear combinations of the position and momentum operators and therefore transform as the normal coordinates: A^+ and A as q_u, B^+ and B as q_v, and similar in case of a T-mode. This is true because no transformations of time are considered here. Since all the excited state functions can be constructed by multiple application of creation operators to the ground state wave function, the transformation properties of $|mn\rangle_{N+1}$ can be found from those of A^+, B^+, and $|m'n'\rangle_N$. This enables us to find symmetry adapted wave functions in successive steps for $N = 1, 2, 3, \ldots$. Note that B^+ is the Hermitian conjugate operator of B and therefore the scalar products with these functions have, for instance, the properties

$$\begin{aligned}\langle lmn \mid l'm' + 1n' \rangle &= (m' + 1)^{-1/2} \langle lmn | B^+ | l'm'n' \rangle \\ &= \left(\frac{m}{m' + 1}\right)^{1/2} \langle lm - 1n \mid l'm'n' \rangle\end{aligned} \tag{5}$$

and so on.

3. *Arrangement of Oscillator Functions*

In case of an E-mode the $N + 1$ oscillator functions belonging to the nth excited state are numbered

$$f_i = |m_i n_i\rangle_N;\ i = 1, 2, 3, \ldots, L_N^E = N + 1 \tag{6}$$

with $m_i = N - i + 1$, $n_i = i - 1$.

In case of T-mode the L_N^T oscillator functions belonging to the Nth excited state are numbered

$$f_i = |l_i m_i n_i\rangle_N;\ i = 1, 2, \ldots, L_N^T = \tfrac{1}{2}(N + 1)(N + 2) \tag{7}$$

with

$$\begin{aligned} i &= (N - l_i)(N + 3 - l_i)\tfrac{1}{2} + 1 - m_i, \\ l_i &= N - I_0, \\ m_i &= \tfrac{1}{2}(I_0 + 1)(I_0 + 2) - i, \\ n_i &= i - \tfrac{1}{2} I_0 (I_0 + 1) - 1, \\ I_0 &= \mathrm{Int}\{\tfrac{1}{2}((8i - 7)^{1/2} - 1)\}, \end{aligned} \tag{8}$$

where Int denotes the integral part of the argument. Equation (8) is also used to find the index i for given values of l_i, m_i, and n_i.

4. *General Description of the Method*

The L_N oscillator functions f_i belonging to an excited state $N > 1$ form a basis of a L_N-dimensional reducible representation of the symmetry group G. If the coordinate system of the three-dimensional vector space is transformed according to an element $s \in G$, the coordinates of the vibrations and the normal coordiantes q change. This leads to a transformed oscillator function which we denote by $P_s f_i$. The representation matrices are then given by the usual scalar product of the elements of the Hilbert space f_i and $P_s f_j$

$$M_s = (P^s_{ij}) \qquad \text{with } P^s_{ij} = (f_i, P_s f_j), \quad i,j = 1, 2,..., L_N. \tag{9}$$

The matrices M_s for $N+1$ can be found from those of the representation matrices of the Nth excited state by a method which is described in detail in the special case of the tetrahedral symmetry group T_d in Sections 6 and 7.

If λ denotes an irreducible representation of G and α a basis function of λ, then the basis functions of the reducible representation M_s which transform as $\lambda\alpha$ can be found from the matrix [3]

$$P^{\lambda\alpha} = \frac{d_\lambda}{n} \sum_{s\in G} d^{\lambda *}_{\alpha\alpha}(s)\, M_s, \tag{10}$$

where n is the (finite) order of the group, d_λ the dimension of the irreducible representation λ, $d^{\lambda *}_{\alpha\alpha}(s)$ is the complex conjugate of the element $\alpha\alpha$ of the matrix of the irreducible representation λ of symmetry element s, and the sum is over all n elements s of the symmetry group G. It can be shown that the eigenvalues of $P^{\lambda\alpha}$ are zero or one and the symmetry adapted wave functions are the eigenfunctions belonging to the eigenvalues one. In order to avoid orthogonalisation procedures for every λ, only functions transforming as $\lambda\alpha$ are obtained this way, the other basis functions of λ can easily be found by multiplying with one of the representation matrices M_s according to Table 1.

The symmetry group G can be generated by products of a certain number of elements $a, b, c, \ldots$. The method to find all symmetry adapted oscillator functions is to

TABLE 1

Transformation Properties of Basis Functions of the Irreducible Representations of the Group T_d

		a	b	c
Γ_1	$A_1 a_1$	a_1	a_1	a_1
Γ_2	$A_2 a_2$	a_2	a_2	$-a_2$
Γ_3	Eu	$-\frac{1}{2}(u + \sqrt{3}v)$	u	u
	Ev	$\frac{1}{2}(\sqrt{3}u - v)$	v	$-v$
Γ_4	$T_1\alpha$	γ	$-\alpha$	$-\beta$
	$T_1\beta$	α	$-\beta$	$-\alpha$
	$T_1\gamma$	β	γ	$-\gamma$
Γ_5	$T_2\xi$	ζ	$-\xi$	η
	$T_2\eta$	ξ	$-\eta$	ξ
	$T_2\zeta$	η	ζ	ζ

construct successively the representation matrices $M_a, M_b, \ldots$, for the group generating elements $a, b, c, \ldots$, for $N+1$ from those of the Nth excited state and to calculate the eigenfunctions of the representation matrices $M_a, M_b, M_c, \ldots$, by numerical methods.

II. Details of the Method for the Tetrahedral Symmetry Group

5. *Tetrahedral Symmetry Group*

The symmetry group T_d of the tetrahedron may be defined by three group generating elements

$$a^3 = b^2 = c^2 = 1, \qquad bab = a^2ba^2, \qquad bc = cb, ac = ca^2, \tag{11}$$

where a is a rotation about $2\pi/3$ along the (111) direction, b a rotation about π along the (001) or z direction, and c is a reflection at a plane perpendicular to the $(-1, 1, 0)$ direction. The definition of the transformation properties of the irreducible representations with respect to a, b, and c is given in Table 1 and is consistent with the definition given by Koster *et al.* [4]. Since the creation operators transform as the corresponding normal coordinates, A^+ and B^+ of an E-mode transform as Eu and Ev, respectively. In case of a T_2-mode A^+, B^+, and C^+ transform as $T_2\xi$, $T_2\eta$, and $T_2\zeta$ of Table 1, respectively.

The oscillator functions f_i for the excited state $N=1$ transform as the corresponding normal coordinates. Table 1 also gives the representation matrices after Eq. (9) for $N=1$

$$E\text{-mode:} \qquad f_1 = |10\rangle_1, \quad f_2 = |01\rangle_1 \quad \text{(Eq. (6))}$$

$$M_a = \tfrac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}; \qquad M_b = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \qquad M_c = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{12}$$

$$T_2\text{-mode:} \qquad f_1 = |100\rangle_1, \quad f_2 = |010\rangle_1, \quad f_3 = |001\rangle_1 \quad \text{(Eq. (7), (8))}$$

$$M_a = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}; \qquad M_b = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \qquad M_c = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{13}$$

Matrices (12) and (13) are used as the starting point from which the representation matrices for $N=2$, $N=3$, and so on can be found by the method described in Sections 6 and 7.

6. *Construction of the Representation Matrices in Case of an E-Mode*

Assume the representation matrices M_s of Eq. (9) for $s = a, b$, and c are known for a fixed value of N. They are generated from the L_N^E functions f_i, $i = 1, 2, \ldots, L_N^E$ defined in Eq. (6). We now consider the system $N+1$ and the corresponding L_{N+1}^E oscillator functions are denoted by ϕ_i. Due to the special arrangement of these functions we have with respect to Eq. (3)

$$\text{for } i = 1, 2, \ldots, L_N^E: \qquad f_i = |m_i n_i\rangle_N, \tag{14}$$
$$\phi_i = |m_i + 1 n_i\rangle_{N+1} = (m_i+1)^{-1/2} A^+ |m_i n_i\rangle_N,$$
$$\text{for } i = L_{N+1}^E: \qquad \phi_i = |0 N+1\rangle_{N+1} = (N+1)^{-1/2} B^+ |0N\rangle_N.$$

We therefore construct the L_{N+1}^E-dimensional representation matrices $\bar{M}_s$ for the system $N+1$ from four submatrices

$$\bar{M}_s = \begin{pmatrix} A_s & B_s \\ C_s & D_s \end{pmatrix}, \tag{15}$$

where A_s is a L_N^E-dimensional square matrix ($i, j = 1, 2, \ldots, L_N^E$)

$$A_s: \qquad (\phi_i, P_s \phi_j) = \langle m_i + 1 n_i | P_s | m_j + 1 n_j \rangle$$
$$= (m_j+1)^{-1/2} \langle m_i + 1 n_i | P_s A^+ | m_j n_j \rangle. \tag{16}$$

In the special cases $s = a, b, c$ we have from Section 2 and Table 1

$$P_a A^+ = \left(-\frac{1}{2} A^+ - \frac{\sqrt{3}}{2} B^+\right) P_a, \qquad P_b A^+ = A^+ P_b, \qquad P_c A^+ = A^+ P_c. \tag{17}$$

This enables us to calculate the matrices A_s from M_s of Eq. (9)

$$A_a: \qquad (\phi_i, P_a \phi_j) = \left(\frac{1}{m_j+1}\right)^{1/2} \langle m_i + 1 n_i | \left(-\frac{1}{2} A^+ - \frac{\sqrt{3}}{2} B^+\right) P_a | m_j n_j \rangle$$
$$= -\frac{1}{2} \left(\frac{m_i+1}{m_j+1}\right)^{1/2} \langle m_i n_i | P_a | m_j n_j \rangle$$
$$- \frac{\sqrt{3}}{2} \left(\frac{n_i}{m_j+1}\right)^{1/2} \langle m_i + 1 n_i - 1 | P_a | m_j n_j \rangle \tag{18}$$
$$= -\frac{1}{2} \left(\frac{m_i+1}{m_j+1}\right)^{1/2} P_{ij}^a - \frac{\sqrt{3}}{2} \left(\frac{n_i}{m_j+1}\right)^{1/2} P_{i-1j}^a,$$

where Eqs. (5) and (6) have been used.

$$A_b: \qquad (\phi_i, P_b \phi_j) = \left(\frac{m_i+1}{m_j+1}\right)^{1/2} P_{ij}^b$$

$$A_c: \qquad (\phi_i, P_c \phi_j) = \left(\frac{m_i+1}{m_j+1}\right)^{1/2} P_{ij}^c.$$

The submatrix B_s of Eq. (15) is a L_N^E by 1-dimensional rectangular matrix $i = 1, 2, \ldots, L_N^E$, $j = L_{N+1}^E$

$$B_s: \qquad (\phi_i, P_s \phi_j) = \langle m_i + 1 n_i | P_s | 0 N+1 \rangle \tag{19}$$
$$= (N+1)^{-1/2} \langle m_i + 1 n_i | P_s B^+ | 0N \rangle.$$

Due to the transformation properties

$$P_a B^+ = (\tfrac{1}{2}\sqrt{3}\,A^+ - \tfrac{1}{2}B^+)\,P_a, \qquad P_b B^+ = B^+ P_b, \qquad P_c B^+ = -B^+ P_c, \tag{20}$$

we find in the same way with $K = L_N^E$

$$\begin{aligned}
B_a: &\quad (\phi_i, P_a\phi_j) = \frac{\sqrt{3}}{2}\left(\frac{m_i+1}{N+1}\right)^{1/2} P^a_{iK} - \frac{1}{2}\left(\frac{n_i}{N+1}\right)^{1/2} P^a_{i-1K},\\
B_b: &\quad (\phi_i, P_b\phi_j) = 0,\\
B_c: &\quad (\phi_i, P_c\phi_j) = 0.
\end{aligned} \tag{21}$$

The submatrix C_s of Eq. (15) is a 1 by L_N^E-dimensional rectangular matrix $i = L_{N+1}^E$, $j = 1, 2,..., L_N^E$ derived in the same way. The result is with $K = L_N^E$

$$\begin{aligned}
C_a: &\quad (\phi_i, P_a\phi_j) = -\frac{\sqrt{3}}{2}\left(\frac{N+1}{m_j+1}\right)^{1/2} P^a_{Kj},\\
C_b: &\quad (\phi_i, P_b\phi_j) = 0,\\
C_c: &\quad (\phi_i, P_c\phi_j) = 0.
\end{aligned} \tag{22}$$

Finally, D_s is given by $(i = j = L_{N+1}^E,\ K = L_N^E)$

$$\begin{aligned}
D_a = (\phi_i, P_a\phi_j) = -\tfrac{1}{2}P^a_{KK}, &\qquad D_b = (\phi_i, P_b\phi_j) = P^b_{KK},\\
D_c = (\phi_i, P_c\phi_j) &= -\,P^c_{KK}.
\end{aligned} \tag{23}$$

Thus the representation matrices $\bar{M}_s$ of Eq. (15) for $N+1$ are found with the help of the matrix elements P^s_{ij} of the representation matrices for N.

7. *Construction of the Representation Matrices in Case of a T_2-Mode*

Assume the representation matrices M_s of Eq. (9) for $s = a, b$, and c are known for a fixed value of N. They are generated from the L_N^T functions f_i, $i = 1, 2,..., L_N^T$ defined in Eqs. (7) and (8). We now consider the system $N+1$ and the corresponding L_{N+1}^T oscillator functions denoted by ϕ_i. Due to the special arrangement of these functions we have with respect to Eq. (4)

$$\begin{aligned}
\text{for } i = 1, 2,..., L_N^T: &\qquad f_i = |l_i m_i n_i\rangle_N\\
&\qquad \phi_i = |l_i + 1 m_i n_i\rangle_{N+1}\\
&\qquad\quad = (l_i+1)^{-1/2} A^+ |l_i m_i n_i\rangle_N,\\
\text{for } i = L_N^T + 1,..., L_{N+1}^T - 1: &\qquad \phi_i = |0 m_i + 1 n_i\rangle_{N+1}\\
&\qquad\quad = (m_i+1)^{-1/2} B^+ |0 m_i n_i\rangle_N,\\
\text{for } i = L_{N+1}^T: &\qquad \phi_i = |00N+1\rangle_{N+1}\\
&\qquad\quad = (N+1)^{-1/2} C^+ |00N\rangle_N.
\end{aligned} \tag{24}$$

Therefore the representation matrices $\bar{M}_s$ for $N+1$ are constructed with the help of nine submatrices which are defined by dividing the oscillator functions ϕ_i in three classes according to Eq. (24)

$$\bar{M}_s = \begin{pmatrix} A_s & B_s & C_s \\ D_s & E_s & F_s \\ G_s & H_s & I_s \end{pmatrix}. \tag{25}$$

The submatrices can be found from the transformation properties of the creation operators taken from Table 1

$$\begin{aligned} P_aA^+ &= C^+P_a, & P_bA^+ &= -A^+P_b, & P_cA^+ &= B^+P_c, \\ P_aB^+ &= A^+P_a, & P_bB^+ &= -B^+P_b, & P_cB^+ &= A^+P_c, \\ P_aC^+ &= B^+P_a, & P_bC^+ &= C^+P_b, & P_cC^+ &= C^+P_c. \end{aligned} \tag{26}$$

The nine submatrices of Eq. (25) are calculated by the same procedure described in Section 6. Using Eqs. (24) and (26) finally gives

$$\begin{aligned}
A_a:&\quad (\phi_i, P_a\phi_j) = \left(\frac{n_i}{l_j+1}\right)^{1/2} \langle l_i+1 m_i n_i-1 | P_a | l_j m_j n_j\rangle, \\
A_b:&\quad (\phi_i, P_b\phi_j) = -\left(\frac{l_i+1}{l_j+1}\right)^{1/2} \langle l_i m_i n_i | P_b | l_j m_j n_j\rangle, \\
A_c:&\quad (\phi_i, P_c\phi_j) = \left(\frac{m_i}{l_j+1}\right)^{1/2} \langle l_i+1 m_i-1 n_i | P_c | l_j m_j n_j\rangle, \\
B_a:&\quad (\phi_i, P_a\phi_j) = \left(\frac{l_i+1}{m_j+1}\right)^{1/2} \langle l_i m_i n_i | P_a | 0 m_j n_j\rangle, \\
B_c:&\quad (\phi_i, P_c\phi_j) = \left(\frac{l_i+1}{m_j+1}\right)^{1/2} \langle l_i m_i n_i | P_c | 0 m_j n_j\rangle, \\
D_a:&\quad (\phi_i, P_a\phi_j) = \left(\frac{n_i}{l_j+1}\right)^{1/2} \langle 0 m_i+1 n_i-1 | P_a | l_j m_j n_j\rangle, \\
D_c:&\quad (\phi_i, P_c\phi_j) = \left(\frac{m_i+1}{l_j+1}\right)^{1/2} \langle 0 m_i n_i | P_c | l_j m_j n_j\rangle, \\
E_b:&\quad (\phi_i, P_b\phi_j) = -\left(\frac{m_i+1}{m_j+1}\right)^{1/2} \langle 0 m_i n_i | P_b | 0 m_j n_j\rangle, \\
F_a:&\quad (\phi_i, P_a\phi_j) = \left(\frac{m_i+1}{N+1}\right)^{1/2} \langle 0 m_i n_i | P_a | 00N\rangle, \\
G_a:&\quad (\phi_i, P_a\phi_j) = \left(\frac{N+1}{l_j+1}\right)^{1/2} \langle 00N | P_a | l_j m_j n_j\rangle, \\
I_b:&\quad (\phi_i, P_b\phi_j) = \langle 00N | P_b | 00N\rangle, \\
I_c:&\quad (\phi_i, P_c\phi_j) = \langle 00N | P_c | 00N\rangle.
\end{aligned} \tag{27}$$

All other submatrices are zero. The corresponding matrix elements of the representation matrices Eq. (9) can easily be found by using Eq. (8).

8. *Results*

A computer program has been written and tested which gives the symmetry adapted oscillator functions for arbitrary excited states N for a two- or three-dimensional oscillator in case of tetrahedral symmetry. As an example Table 2 gives the results for a T_2 oscillator up to $N=6$. In case of an E-oscillator symmetry adapted wave functions up to $N=6$ can be found in [1].

TABLE 2

Symmetry Adapted Wave Functions of a Three-Dimensional Harmonic Oscillator of Symmetry T_2

N	A_1	A_2	Eu	Ev
0	$\|000\rangle : 1$			
2	$\|200\rangle : 1/\sqrt{3}$		$\|200\rangle : -1/\sqrt{6}$	$\|200\rangle : 1/\sqrt{2}$
	$\|020\rangle : 1/\sqrt{3}$		$\|020\rangle : -1/\sqrt{6}$	$\|020\rangle : -1/\sqrt{2}$
	$\|002\rangle : 1/\sqrt{3}$		$\|002\rangle : 2/\sqrt{6}$	
3	$\|111\rangle : 1$			
4	$\|400\rangle : 1/\sqrt{3}$		$\|400\rangle : -1/\sqrt{6}$	$\|400\rangle : 1/\sqrt{2}$
	$\|040\rangle : 1/\sqrt{3}$		$\|040\rangle : -1/\sqrt{6}$	$\|040\rangle : -1/\sqrt{2}$
	$\|004\rangle : 1/\sqrt{3}$		$\|004\rangle : 2/\sqrt{6}$	
	$\|220\rangle : 1/\sqrt{3}$		$\|220\rangle : 2/\sqrt{6}$	
	$\|202\rangle : 1/\sqrt{3}$		$\|202\rangle : -1/\sqrt{6}$	$\|202\rangle : -1/\sqrt{2}$
	$\|022\rangle : 1/\sqrt{3}$		$\|022\rangle : -1/\sqrt{6}$	$\|022\rangle : 1/\sqrt{2}$
5	$\|311\rangle : 1/\sqrt{3}$		$\|311\rangle : -1/\sqrt{6}$	$\|311\rangle : 1/\sqrt{2}$
	$\|131\rangle : 1/\sqrt{3}$		$\|131\rangle : -1/\sqrt{6}$	$\|131\rangle : -1/\sqrt{2}$
	$\|113\rangle : 1/\sqrt{3}$		$\|113\rangle : 2/\sqrt{6}$	
6	$\|420\rangle : 1/\sqrt{6}$	$\|420\rangle : 1/\sqrt{6}$	$\|420\rangle : 1/\sqrt{12}$	$\|420\rangle : -1/2$
	$\|402\rangle : 1/\sqrt{6}$	$\|402\rangle : -1/\sqrt{6}$	$\|402\rangle : 1/\sqrt{12}$	$\|402\rangle : -1/2$
	$\|240\rangle : 1/\sqrt{6}$	$\|240\rangle : -1/\sqrt{6}$	$\|240\rangle : 1/\sqrt{12}$	$\|240\rangle : 1/2$
	$\|204\rangle : 1/\sqrt{6}$	$\|204\rangle : 1/\sqrt{6}$	$\|204\rangle : -1/\sqrt{3}$	$\|042\rangle : 1/2$
	$\|042\rangle : 1/\sqrt{6}$	$\|042\rangle : 1/\sqrt{6}$	$\|042\rangle : 1/\sqrt{12}$	
	$\|024\rangle : 1/\sqrt{6}$	$\|024\rangle : -1/\sqrt{6}$	$\|024\rangle : -1/\sqrt{3}$	
	$\|600\rangle : 1/\sqrt{3}$		$\|420\rangle\ -1/2$	$\|420\rangle : -1/\sqrt{12}$
	$\|060\rangle : 1/\sqrt{3}$		$\|402\rangle\ 1/2$	$\|402\rangle : 1/\sqrt{12}$
	$\|006\rangle : 1/\sqrt{3}$		$\|240\rangle\ -1/2$	$\|240\rangle : 1/\sqrt{12}$
			$\|042\rangle\ 1/2$	$\|204\rangle : 1/\sqrt{3}$
				$\|042\rangle : -1/\sqrt{12}$
				$\|024\rangle : -1/\sqrt{3}$
	$\|222\rangle : 1$		$\|600\rangle : -1/\sqrt{6}$	$\|600\rangle : 1/\sqrt{2}$
			$\|060\rangle : -1/\sqrt{6}$	$\|060\rangle : -1/\sqrt{2}$
			$\|006\rangle : 2/\sqrt{6}$	

Table continued

TABLE 2 (*continued*)

N	$T_1\alpha$	$T_1\beta$	$T_1\gamma$
3	$\|120\rangle: 1/\sqrt{2}$ $\|102\rangle: -1/\sqrt{2}$	$\|210\rangle: -1/\sqrt{2}$ $\|012\rangle: 1/\sqrt{2}$	$\|210\rangle: 1/\sqrt{2}$ $\|021\rangle: -1/\sqrt{2}$
4	$\|031\rangle: -1/\sqrt{2}$ $\|013\rangle: 1/\sqrt{2}$	$\|301\rangle: 1/\sqrt{2}$ $\|103\rangle: -1/\sqrt{2}$	$\|301\rangle: -1/\sqrt{2}$ $\|130\rangle: 1/\sqrt{2}$
5	$\|320\rangle: -1/\sqrt{2}$ $\|302\rangle: 1/\sqrt{2}$ $\|140\rangle: 1/\sqrt{2}$ $\|104\rangle: -1/\sqrt{2}$	$\|230\rangle: 1/\sqrt{2}$ $\|032\rangle: -1/\sqrt{2}$ $\|410\rangle: -1/\sqrt{2}$ $\|041\rangle: 1/\sqrt{2}$	$\|203\rangle: -1/\sqrt{2}$ $\|023\rangle: 1/\sqrt{2}$ $\|401\rangle: 1/\sqrt{2}$ $\|041\rangle: -1/\sqrt{2}$
6	$\|231\rangle: 1/\sqrt{2}$ $\|213\rangle: -1/\sqrt{2}$ $\|051\rangle: 1/\sqrt{2}$ $\|015\rangle: -1/\sqrt{2}$	$\|321\rangle: -1/\sqrt{2}$ $\|123\rangle: 1/\sqrt{2}$ $\|501\rangle: -1/\sqrt{2}$ $\|105\rangle: 1/\sqrt{2}$	$\|312\rangle: 1/\sqrt{2}$ $\|132\rangle: -1/\sqrt{2}$ $\|510\rangle: 1/\sqrt{2}$ $\|150\rangle: -1/\sqrt{2}$

N	$T_2\xi$	$T_2\eta$	$T_2\zeta$
1	$\|100\rangle: 1$	$\|010\rangle: 1$	$\|001\rangle: 1$
2	$\|011\rangle: 1$	$\|101\rangle: 1$	$\|110\rangle: 1$
3	$\|300\rangle: 1$ $\|120\rangle: 1/\sqrt{2}$ $\|102\rangle: 1/\sqrt{2}$	$\|030\rangle: 1$ $\|210\rangle: 1/\sqrt{2}$ $\|012\rangle: 1/\sqrt{2}$	$\|003\rangle: 1$ $\|201\rangle: 1/\sqrt{2}$ $\|021\rangle: 1/\sqrt{2}$
4	$\|211\rangle: 1$ $\|031\rangle: 1/\sqrt{2}$ $\|013\rangle: 1/\sqrt{2}$	$\|121\rangle: 1$ $\|301\rangle: 1/\sqrt{2}$ $\|103\rangle: 1/\sqrt{2}$	$\|112\rangle: 1$ $\|310\rangle: 1/\sqrt{2}$ $\|130\rangle: 1/\sqrt{2}$
5	$\|500\rangle: 1$ $\|140\rangle: 1/\sqrt{2}$ $\|104\rangle: 1/\sqrt{2}$ $\|320\rangle: 1/\sqrt{2}$ $\|302\rangle: 1/\sqrt{2}$ $\|122\rangle: 1$	$\|050\rangle: 1$ $\|410\rangle: 1/\sqrt{2}$ $\|014\rangle: 1/\sqrt{2}$ $\|230\rangle: 1/\sqrt{2}$ $\|032\rangle: 1/\sqrt{2}$ $\|212\rangle: 1$	$\|005\rangle: 1$ $\|401\rangle: 1/\sqrt{2}$ $\|041\rangle: 1/\sqrt{2}$ $\|203\rangle: 1/\sqrt{2}$ $\|023\rangle: 1/\sqrt{2}$ $\|221\rangle: 1$
6	$\|231\rangle: -1/\sqrt{2}$ $\|213\rangle: -1/\sqrt{2}$ $\|051\rangle: -1/\sqrt{2}$ $\|015\rangle: -1/\sqrt{2}$ $\|411\rangle: 1$ $\|033\rangle: 1$	$\|321\rangle: -1/\sqrt{2}$ $\|123\rangle: -1/\sqrt{2}$ $\|501\rangle: -1/\sqrt{2}$ $\|105\rangle: -1/\sqrt{2}$ $\|141\rangle: 1$ $\|303\rangle: 1$	$\|312\rangle: -1/\sqrt{2}$ $\|132\rangle: -1/\sqrt{2}$ $\|510\rangle: -1/\sqrt{2}$ $\|150\rangle: -1/\sqrt{2}$ $\|114\rangle: 1$ $\|330\rangle: 1$

Note. $|lmn\rangle$ is a function with l phonons of type ξ, m phonons of type η, and n phonons of type ζ. (For example, $(2/\sqrt{6})|220\rangle - (1|\sqrt{6})|202\rangle - (1/\sqrt{6})|022\rangle$ and $-(1/\sqrt{2})|202\rangle + (1/\sqrt{2})|022\rangle$ transform as u and v of the irreducible representation E.)

For the $T_2(E)$ oscillator a calculation up to $N = 10$ (14) has been performed. To find the 286 (120) symmetry adapted functions the CYBER 170 calculator used 309 (9) sec execution time and the memory used was about 80 K (38 K).

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