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Clebsch-Gordan coefficients for $M \times M$ in beta tungsten

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Résumé. — On calcule les coefficients de Clebsch-Gordan pour les représentations irréductibles $M \times M$ de la structure du bêta-tungstène.

Abstract. — The Clebsch-Gordan coefficients are calculated for $M \times M$ irreducible representations in the beta tungsten structure.

1. **Introduction.** — The binary intermetallic compounds having A_3B composition and the β -tungsten or A-15 structure are of significant theoretical interest and outstanding practical importance. Compounds such as Nb_3Ge , Nb_3Sn , Nb_3Al , V_3Ga , V_3Si , crystallizing in A-15 structure possess the highest transition temperatures to the superconducting state that have been observed [1-6].

Theories of structural phase transitions, applied to A-15 compounds, were proposed by Birman [7] and Gorkov [8] and discussed in [9-13]. In several compounds with the A-15 structure the phonons at the M point of the Brillouin zone become soft leading to lattice instability and eventually to a distortive phase transition [14].

In recent years much attention has been directed to the Clebsch-Gordan (CG) coefficients of the crystallographic space group representations. In particular Birman *et al.* [15-17] have shown that the matrix elements of the first order scattering tensors are precisely certain CG coefficients or prescribed linear combinations, the elements of the second order tensor are particular sums of products of CG coefficients. The matrix elements of the effective Hamiltonian are products of appropriate CG coefficients times symmetrized tensorial field quantities [18].

The calculation of CG coefficients for space groups can be done by several methods [17, 19-25]. For a computation of CG coefficients or scattering tensors an elaboration of the selection rules is a first necessary step. The selection rules for the double space group

$O_h^3(Pm3n)$ of the A-15 structure have been determined [26, 27] and checked with an output of the computer program written for determining the reduction of the Kronecker products of the irreducible representations of crystallographic space groups [28, 29].

The present paper deals with the problem of constructing basis functions for the representations which are contained in the Kronecker product of two irreducible space group representations. We computed the CG coefficients of the single-valued representations $X \times X$, $M \times M$ and $R \times R$ for the space group O_h^3 [30].

2. **Calculation of the Clebsch-Gordan coefficients using matrix elements of small representations.** — For the crystallographic space group representations with wave vectors \mathbf{k}_σ , $\mathbf{k}'_{\sigma'}$, $\mathbf{k}''_{\sigma''}$ satisfying wave vector selection rules

$$\mathbf{k}_\sigma + \mathbf{k}'_{\sigma'} = \mathbf{k}''_{\sigma''} \quad (1)$$

the Clebsch-Gordan coefficients

$$U_{\sigma\sigma'a',\mathbf{k}''\mathbf{l}''\gamma\sigma''a''}^{\mathbf{k}(l)\otimes\mathbf{k}'(l')} = U_{\sigma\sigma'a',\sigma''a''}^\gamma = \begin{pmatrix} \mathbf{k} & l & \mathbf{k}' & l' & \mathbf{k}'' & l'' & \gamma \\ \sigma & a & \sigma' & a' & \sigma'' & a'' & \end{pmatrix} \quad (2)$$

are defined as coefficients between the basis functions $\Psi_a^{\mathbf{k}''\mathbf{l}''\gamma}$ and $\Phi_a^{\mathbf{k}\sigma l} \Psi_a^{\mathbf{k}'\sigma' l'}$ of the representations of dimensions $\dim(l'')$ and $\dim(l) \times \dim(l')$ respectively

$$\Psi_{a''\sigma''l''\gamma}^{\mathbf{k}} = \sum_{\sigma a} \sum_{\sigma' a'} \left(\begin{array}{c|c} \mathbf{k} & l \\ \sigma & a \end{array} \begin{array}{c|c} \mathbf{k}' & l' \\ \sigma' & a' \end{array} \middle| \begin{array}{c|c} \mathbf{k}'' & l'' \\ \sigma'' & a'' \end{array} \begin{array}{c} \gamma \end{array} \right) \times \\ \times \Phi_a^{\mathbf{k}\sigma l} \Psi_{a''\sigma''l''}^{\mathbf{k}'\sigma' l'}. \quad (3)$$

Berenson, Birman *et al.* [21, 22] have shown that the CG coefficients for representations of a space group can be calculated from the small irreducible representations $d^{\mathbf{k}l}$, $d^{\mathbf{k}'l'}$, $d^{\mathbf{k}''l''}$ of the little wave vector groups [31].

The block of CG coefficients for $\sigma = \sigma' = \sigma'' = 1$ can be calculated from

$$U_{1a1a'1a''} U_{1\bar{a}1\bar{a}'1\bar{a}''}^* = \frac{\dim(l'')}{h} \sum_S d^{\mathbf{k}l} (\{\varphi_S | \tau_S\})_{a\bar{a}} \times \\ \times d^{\mathbf{k}'l'} (\{\varphi_S | \tau_S\})_{a'\bar{a}'} d^{\mathbf{k}''l''} (\{\varphi_S | \tau_S\})_{a''\bar{a}''}. \quad (4)$$

Here h is the order of the wave vector group of \mathbf{k}'' and the summation runs over

$$\{\varphi_S | \tau_S\} \in G^{\mathbf{k}} \wedge G^{\mathbf{k}'} \wedge G^{\mathbf{k}''},$$

i.e. the intersection of the wave vector groups of \mathbf{k} , \mathbf{k}' and \mathbf{k}'' satisfying wave vector selection rule of eq. (1).

The $(\sigma, \sigma', \sigma'')$ blocks of CG coefficients are obtained from the U_{111} block by matrix multiplication

$$U_{\sigma b\sigma' b', l''\gamma\sigma'' b''}^{l \otimes l'} = \sum_a \sum_{a'} \sum_{a''} [d^{\mathbf{k}l} (\{\varphi_{\mathbf{k}} | \mathbf{t}_{\mathbf{k}}\}) \times \\ \times d^{\mathbf{k}'l'} (\{\varphi_{\mathbf{k}'} | \mathbf{t}_{\mathbf{k}'}\})]_{bb'aa'} \times \\ \times U_{1a'1a''1a}^{l \otimes l'} d^{\mathbf{k}''l''} (\{\varphi_{\mathbf{k}''} | \mathbf{t}_{\mathbf{k}''}\})_{a''b''}^{-1} \quad (5)$$

where the canonical wave vectors satisfy $\mathbf{k} + \mathbf{k}' = \mathbf{k}''$ modulo a vector of the reciprocal lattice, and

$$\{\varphi_{\sigma} | \tau_{\sigma}\} \{\varphi_{\mathbf{k}} | \mathbf{t}_{\mathbf{k}}\} = \{\varphi_{\sigma'} | \tau_{\sigma'}\} \{\varphi_{\mathbf{k}'} | \mathbf{t}_{\mathbf{k}'}\} = \\ = \{\varphi_{\sigma''} | \tau_{\sigma''}\} \{\varphi_{\mathbf{k}''} | \mathbf{t}_{\mathbf{k}''}\} = \{\varphi_{\Sigma} | \tau_{\Sigma}\}. \quad (6)$$

Here $\{\varphi_{\Sigma} | \tau_{\Sigma}\}$ is one space group operation which rotates the $(1, 1, 1)$ block into $(\sigma, \sigma', \sigma'')$ block so that

$$\varphi_{\Sigma} \mathbf{k} = \mathbf{k}_{\sigma}, \quad \varphi_{\Sigma} \mathbf{k}' = \mathbf{k}'_{\sigma'}, \quad \varphi_{\Sigma} \mathbf{k}'' = \mathbf{k}''_{\sigma''}. \quad (7)$$

The translations $\mathbf{t}_{\mathbf{k}} = \tau_{\sigma} + \mathbf{R}_{\mathbf{L}}$ where τ_{σ} is a fractional translation in eq. (6) and $\mathbf{R}_{\mathbf{L}}$ is a lattice vector.

3. Clebsch-Gordan coefficients for $M \times M$ in O_h^3 . — We compute the Clebsch-Gordan coefficients for the single-valued representations of the nonsymmorphic space group $O_h^3(\text{Pm}3n)$. We use the Miller and Love (M-L) [32] numbering of the space group symmetry operations as given for the cubic group in their table I on p. 123, and M-L canonical wave vectors, given on p. 129. We use M-L irreducible representations of the wave vector groups, computed from the M-L generators by a computer program [33].

3.1 $M \times M$. — We use $\mathbf{k}_M = (1, 1, 0) \pi/a_L$ as the first M wave vector, see table I. The space group O_h^3

Table I. — Coordinates of the wave vectors to the symmetry points of the Brillouin zone, a_L is the cubic lattice constant.

	\mathbf{k}
Γ	(0, 0, 0)
X	(0, 1, 0) π/a_L
M	(1, 1, 0) π/a_L
R	(1, 1, 1) π/a_L

can be decomposed into cosets with respect to $G(M) = G^{\mathbf{k}_M}$

$$O_h^3 = \{1 | 0\} G(M) + \{5 | 0\} G(M) + \\ + \{9 | 0\} G(M) = \sum_{\sigma=1}^3 \{\varphi_{\sigma} | \tau_{\sigma}\} G(M). \quad (8)$$

The wave vectors satisfying the selection rule $\mathbf{k}_M + \mathbf{k}_M = \mathbf{k}_\Gamma$ of table II are shown in table III. From the vectors

$$\mathbf{k} = \mathbf{k}_{\sigma=1} = \mathbf{k}_M, \quad \mathbf{k}' = \mathbf{k}'_{\sigma'=1} = \mathbf{k}_M, \\ \mathbf{k}'' = \mathbf{k}''_{\sigma''=1} = \mathbf{k}_\Gamma \quad (9)$$

Table II. — Leading wave vector selection rules, LWVSRs, and intersections of the wave vector groups of O_h^3 .

LWVSR	Intersection
$\mathbf{k} + \mathbf{k}' = \mathbf{k}''$	$G^{\mathbf{k}} \wedge G^{\mathbf{k}'} \wedge G^{\mathbf{k}''}$
$\mathbf{k}_X + \mathbf{k}_X = \mathbf{k}_\Gamma$	$G^{\mathbf{k}_X}$
$\mathbf{k}_X + 5 \mathbf{k}_X = \mathbf{k}_M$	$\{1, 2, 3, 4, 25, 26, 27, 28\}$
$\mathbf{k}_M + \mathbf{k}_M = \mathbf{k}_\Gamma$	$G^{\mathbf{k}_M}$
$5 \mathbf{k}_M + 9 \mathbf{k}_M = \mathbf{k}_M$	$\{1, 2, 3, 4, 25, 26, 27, 28\}$
$\mathbf{k}_R + \mathbf{k}_R = \mathbf{k}_\Gamma$	$G^{\mathbf{k}_R}$

and from coset representatives of eq. (8) the space operations $\{\varphi_{\Sigma} | \tau_{\Sigma}\}$ and $\{\varphi_{\mathbf{k}} | \mathbf{t}_{\mathbf{k}}\}$, $\{\varphi_{\mathbf{k}'} | \mathbf{t}_{\mathbf{k}'}\}$, $\{\varphi_{\mathbf{k}''} | \mathbf{t}_{\mathbf{k}''}\}$ are calculated and are shown in table III.

The first wave vectors satisfying the selection rule $5 \mathbf{k}_M + 9 \mathbf{k}_M = \mathbf{k}_M$ are as shown in table III,

$$\varphi_{\sigma} \mathbf{k} = \mathbf{k}_{\sigma=1} = 5 \mathbf{k}_M, \quad \varphi_{\sigma'} \mathbf{k}' = \mathbf{k}'_{\sigma'=1} = 9 \mathbf{k}_M, \\ \varphi_{\sigma''} \mathbf{k}'' = \mathbf{k}''_{\sigma''=1} = \mathbf{k}_M. \quad (10)$$

Hence for channel M we have now

$$\varphi_{\sigma} \mathbf{k} = 5 \mathbf{k}_M \\ \varphi_{\sigma'} \mathbf{k}' = 9 \mathbf{k}_M \\ \varphi_{\sigma''} \mathbf{k}'' = \mathbf{k}_M. \quad (11)$$

We transform by these space operations the small representations [26, 27]

$$d^{(\varphi_{\sigma} \mathbf{k})l} (\{\varphi_S | \mathbf{t}_S\}) = \\ = d^{\mathbf{k}l} (\{\varphi_{\sigma} | \tau_{\sigma}\}^{-1} \{\varphi_S | \mathbf{t}_S\} \{\varphi_{\sigma} | \tau_{\sigma}\})$$

$$d^{(\varphi_{\sigma'} \mathbf{k}')'}(\{\varphi_S | \mathbf{t}_S\}) = d^{k'l'}(\{\varphi_{\sigma'} | \tau_{\sigma'}\}^{-1} \{\varphi_S | \mathbf{t}_S\} \{\varphi_{\sigma'} | \tau_{\sigma'}\}) \quad (12)$$

$$d^{(\varphi_{\sigma''} \mathbf{k}'')'}(\{\varphi_S | \mathbf{t}_S\}) = d^{k''l''}(\{\varphi_{\sigma''} | \tau_{\sigma''}\}^{-1} \{\varphi_S | \mathbf{t}_S\} \{\varphi_{\sigma''} | \tau_{\sigma''}\}).$$

Thus in the summation in eq. (4) the ordered group elements in the first factor, transformed from d^{kl} , are d^{k^m} (1, 3, 4, 2, 25, 27, 28, 26), in the second factor, transformed from $d^{k'l'}$, are d^{k^m} (1, 4, 2, 3, 25, 28, 26, 27), and in the third factor, transformed from $d^{k''l''}$, are d^{k^m} (1, 2, 3, 4, 25, 26, 27, 28). We perform summation on the right-hand side of eq. (4) and we obtain the U_{111} block of the CG coefficients.

The operations $\{\varphi_{\sigma} | \tau_{\sigma}\}$ and $\{\varphi_{\mathbf{k}} | \mathbf{t}_{\mathbf{k}}\}$, $\{\varphi_{\mathbf{k}'} | \mathbf{t}_{\mathbf{k}'}\}$, $\{\varphi_{\mathbf{k}''} | \mathbf{t}_{\mathbf{k}''}\}$ calculated from the coset representatives of eq. (8) and from the wave vectors of eq. (9) and (10), are shown in table III. There the third column which follows from the wave vector selection rules gives the indices $\sigma\sigma'\sigma''$ numbering the blocks of CG coefficients. The fourth column in table III gives a separate numbering in channel M. There are in channel Γ three blocks of CG coefficients given in tables IV and V, orthogonal to six blocks in channel M, given in tables IV and VI. The computed CG coefficients for $M_j \times M_j$ ($j = 1, 2, 3, 4$) have been checked by the Sakata method [20]. For numbering the CG coefficients of the full group

representations $M_{5\pm} \times M_{5\pm}$ we use in tables V and VI an additional, second, set of indices $\alpha\alpha'\alpha''$ obtained by adding 3 to the first set.

3.2 DESCRIPTION OF TABLES OF CG COEFFICIENTS. — In the tables of CG coefficients we use

$$a = 1/\sqrt{2}, \quad b = 1/\sqrt{3},$$

$$c = \omega/\sqrt{3} = (1/\sqrt{3}) \exp(2\pi i/3) = (3i - \sqrt{3})/6, \quad (13)$$

$$d = 1/\sqrt{6}.$$

In table VI the entries not written explicitly are zero.

4. Use of tables. — The tables of CG coefficients can be used to obtain symmetrized linear combinations of products of basis wave functions [17, 22, 34, 35].

For space group representations $D^{k^{(l)}}$, with basis functions $\phi_{\sigma\alpha}^{k^{(l)}}$, and $D^{k^{(l')}}$, with basis $\psi_{\sigma'\alpha'}^{k^{(l)'}}$, whose Kronecker product $D^{k^{(l)}} \otimes D^{k^{(l)'}}$ contains up to several times the representation $D^{k^{(l'')}}$, with basis $\Psi_{\sigma''\alpha''}^{k^{(l)'}}$, one basis function $\Psi_{\sigma''\alpha''}^{k^{(l)'}}$ can be expressed according to eq. (3).

As a particular example we give the symmetrized linear combinations of products of basis functions which occur in

$$X_1 \times X_1 = [\Gamma_{1+} + \Gamma_{2+} + 2\Gamma_{3+} + \Gamma_{5-}] + \Gamma_{4-}.$$

Table III. — Wave vector selection rules and the symmetry operations for calculating the $(\sigma, \sigma', \sigma'')$ blocks of Clebsch-Gordan coefficients for $M \times M$.

	$\sigma\sigma'\sigma''$	$\{\varphi_{\sigma} \tau_{\sigma}\}$	$\{\varphi_{\mathbf{k}} \mathbf{t}_{\mathbf{k}}\}$	$\{\varphi_{\mathbf{k}'} \mathbf{t}_{\mathbf{k}'}\}$	$\{\varphi_{\mathbf{k}''} \mathbf{t}_{\mathbf{k}''}\}$
$\mathbf{k}_M + \mathbf{k}_M = \mathbf{k}_{\Gamma}$	Γ 1 1 1	{ 1 0 }	{ 1 0 }	{ 1 0 }	{ 1 0 }
$5 \mathbf{k}_M + 5 \mathbf{k}_M = \mathbf{k}_{\Gamma}$	2 2 1	{ 5 0 }	{ 1 0 }	{ 1 0 }	{ 1 0 }
$9 \mathbf{k}_M + 9 \mathbf{k}_M = \mathbf{k}_{\Gamma}$	3 3 1	{ 9 0 }	{ 1 0 }	{ 1 0 }	{ 1 0 }
$5 \mathbf{k}_M + 9 \mathbf{k}_M = \mathbf{k}_M$	M 2 3 1	{ 1 0 }	{ 1 0 }	{ 1 0 }	{ 1 0 }
$9 \mathbf{k}_M + \mathbf{k}_M = 5 \mathbf{k}_M$	3 1 2	{ 5 0 }	{ 1 0 }	{ 1 0 }	{ 1 0 }
$\mathbf{k}_M + 5 \mathbf{k}_M = 9 \mathbf{k}_M$	1 2 3	{ 9 0 }	{ 1 0 }	{ 1 0 }	{ 1 0 }
$9 \mathbf{k}_M + 5 \mathbf{k}_M = \mathbf{k}_M$	3 2 1	{ 13 τ }	{ 21 τ }	{ 17 τ }	{ 13 τ }
$\mathbf{k}_M + 9 \mathbf{k}_M = 5 \mathbf{k}_M$	1 3 2	{ 17 τ }	{ 21 τ }	{ 17 τ }	{ 13 τ }
$5 \mathbf{k}_M + \mathbf{k}_M = 9 \mathbf{k}_M$	2 1 3	{ 21 τ }	{ 21 τ }	{ 17 τ }	{ 13 τ }

$\tau = (1/2, 1/2, 1/2) a_1$

Table IV. — Clebsch-Gordan coefficients for $M_i \times M_i$ ($i = 1^{\pm}, 2^{\pm}$) and $M_j \times M_j$ ($j = 3^{\pm}, 4^{\pm}$).

$M_i \times M_i$	$M_j \times M_j$	$\sigma \sigma' \sigma''$	$\alpha \alpha'$	$\alpha'' =$	1	1	2	1	2	3	1	2	3
Γ	Γ	1 1 1	1 1		b	b	b	0	0	0	0	0	0
Γ	Γ	2 2 1	2 2		b	c	c^*	0	0	0	0	0	0
Γ	Γ	3 3 1	3 3		b	c^*	c	0	0	0	0	0	0
M	M	2 3 1	2 3		0	0	0	a	0	0	a	0	0
M	M	3 2 1	3 2		0	0	0	a	0	0	$-a$	0	0
M	M	1 3 2	1 3		0	0	0	0	a	0	0	$-a$	0
M	M	3 1 2	3 1		0	0	0	0	a	0	0	a	0
M	M	1 2 3	1 2		0	0	0	0	0	a	0	0	a
M	M	2 1 3	2 1		0	0	0	0	0	a	0	0	$-a$

Table V. — Clebsch-Gordan coefficients for $M_{5\pm} \times M_{5\pm}$.

$M_{5\pm} \times M_{5\pm}$ $\sigma \ \sigma' \ \sigma''$	=	$\alpha \ \alpha'$	$\alpha'' =$	$[\Gamma_{1+}] +$		$\Gamma_{2+} +$		$\Gamma_{3+} +$		$\Gamma_{4+} +$			$[\Gamma_{5+}]$			
				1	1	1	2	1	2	1	2	3	1	2	3	
1 1 1	=	1 1	1	d	d	b	0	0	b	0	0	0	0	0	0	
				1 4	0	0	0	0	0	0	a	0	0	a	0	0
				4 1	0	0	0	0	0	0	$-a$	0	0	a	0	0
2 2 1	=	2 2	2	d	$-d$	0	b	b	0	0	0	0	0	0	0	
				2 5	0	0	0	0	0	0	0	0	a	0	0	a
				5 2	0	0	0	0	0	0	0	0	$-a$	0	0	a
3 3 1	=	3 3	3	d	$-d$	0	c^*	c	0	0	0	0	0	0	0	
				3 6	0	0	0	0	0	0	0	a	0	0	a	0
				6 3	0	0	0	0	0	0	0	$-a$	0	0	a	0
				6 6	d	$-d$	0	c	c^*	0	0	0	0	0	0	0

Table VI. — Clebsch-Gordan coefficients for $M_{5\pm} \times M_{5\pm}$.

$M_{5\pm} \times M_{5\pm}$ $\sigma \ \sigma' \ \sigma''$	=	$\alpha \ \alpha'$	$\alpha'' =$	$[M_{1+}] +$			$M_{2+} +$			$M_{3+} +$			$[M_{4+}] +$						M_{5+}								
				1	2	3	1	2	3	1	2	3	1	2	3	4	5	6	1	2	3	4	5	6			
2 3 1	=	2 3	2	0	0				0	0	0	0	1	0			0	0									
				2 6	a	a				0	0	0	0	0	0	0			0	0							
				5 3	0	0				a	a	0	0	0	0	0			0	0							
3 2 1	=	3 2	3	0	0				0	0	0	0	0			0	0										
				3 5	0	0				0	0	$-a$	a	0	0			0	0								
				6 2	a	$-a$				0	0	0	0	0	0			0	0								
1 3 2	=	1 3	1	0	0				0	0	0	0	0			0	0										
				1 6	0	0				$-a$	a	0	0	0	0			0	0								
				4 3	a	$-a$				0	0	0	0	0	0			0	0								
3 1 2	=	3 1	3	0	0				0	0	0	0	1	0			0	0									
				3 4	a	a				0	0	0	0	0	0			0	0								
				6 1	0	0				a	a	0	0	0	0			0	0								
1 2 3	=	1 2	1	0	0				0	0	0	0	0			0	0										
				1 5	a	a				0	0	0	0	0	0			0	0								
				4 2	0	0				a	a	0	0	0	0			0	0								
2 1 3	=	2 1	2	0	0				0	0	0	0	0			0	0										
				2 4	0	0				0	0	$-a$	a	0	0			0	0								
				5 1	a	$-a$				0	0	0	0	0	0			0	0								
5 4	=	5 4	5	0	0				0	0	0	0	0			0	0										

From table VII of reference [30] we have

$$\Psi_{11}^{k[\Gamma_{1+}]} = \frac{1}{\sqrt{6}} (\Phi_{11}^{k(X_1)} \Psi_{11}^{k(X_1)} + \Phi_{14}^{k(X_1)} \Psi_{14}^{k(X_1)} + \Phi_{22}^{k(X_1)} \Psi_{22}^{k(X_1)} + \Phi_{25}^{k(X_1)} \Psi_{25}^{k(X_1)} + \Phi_{33}^{k(X_1)} \Psi_{33}^{k(X_1)} + \Phi_{36}^{k(X_1)} \Psi_{36}^{k(X_1)})$$

$$\Psi_{11}^{k[\Gamma_{2+}]} = \frac{1}{\sqrt{6}} (\Phi_{11}^{k(X_1)} \Psi_{11}^{k(X_1)} - \Phi_{14}^{k(X_1)} \Psi_{14}^{k(X_1)} + \Phi_{22}^{k(X_1)} \Psi_{22}^{k(X_1)} - \Phi_{25}^{k(X_1)} \Psi_{25}^{k(X_1)} + \Phi_{33}^{k(X_1)} \Psi_{33}^{k(X_1)} - \Phi_{36}^{k(X_1)} \Psi_{36}^{k(X_1)})$$

For the two-dimensional representation Γ_{3+} occurring twice, the basis functions are

$$\Psi_{11}^{k[\Gamma_{3+1}]} = \frac{1}{\sqrt{3}} (\Phi_{11}^{k(X_1)} \Psi_{11}^{k(X_1)} + \omega \Phi_{22}^{k(X_1)} \Psi_{22}^{k(X_1)} + \omega^2 \Phi_{33}^{k(X_1)} \Psi_{33}^{k(X_1)})$$

$$\Psi_{12}^{k[\Gamma_{3+1}]} = \frac{1}{\sqrt{3}} (\omega \Phi_{14}^{k(X_1)} \Psi_{14}^{k(X_1)} + \Phi_{25}^{k(X_1)} \Psi_{25}^{k(X_1)} + \omega^2 \Phi_{36}^{k(X_1)} \Psi_{36}^{k(X_1)})$$

$$\Psi_{11}^{k(\Gamma_{3+}^{12})} = \frac{1}{\sqrt{3}} (\omega^2 \Phi_{14}^{k(X_1)} \Psi_{14}^{k(X_1)} + \Phi_{25}^{k(X_1)} \Psi_{25}^{k(X_1)} + \omega \Phi_{36}^{k(X_1)} \Psi_{36}^{k(X_1)})$$

$$\Psi_{12}^{k(\Gamma_{3+}^{12})} = \frac{1}{\sqrt{3}} (\Phi_{11}^{k(X_1)} \Psi_{11}^{k(X_1)} + \omega^2 \Phi_{22}^{k(X_1)} \Psi_{22}^{k(X_1)} + \omega \Phi_{33}^{k(X_1)} \Psi_{33}^{k(X_1)}).$$

For the three-dimensional representations Γ_{4-} and Γ_{5-} the basis functions are

$$\Psi_{11}^{k(\Gamma_{4-})} = \frac{1}{\sqrt{2}} (\Phi_{33}^{k(X_1)} \Psi_{36}^{k(X_1)} - \Phi_{36}^{k(X_1)} \Psi_{33}^{k(X_1)})$$

$$\Psi_{12}^{k(\Gamma_{4-})} = \frac{1}{\sqrt{2}} (\Phi_{22}^{k(X_1)} \Psi_{25}^{k(X_1)} - \Phi_{25}^{k(X_1)} \Psi_{22}^{k(X_1)})$$

$$\Psi_{13}^{k(\Gamma_{4-})} = \frac{1}{\sqrt{2}} (\Phi_{11}^{k(X_1)} \Psi_{14}^{k(X_1)} - \Phi_{14}^{k(X_1)} \Psi_{11}^{k(X_1)})$$

$$\Psi_{11}^{k(\Gamma_{5-})} = \frac{1}{\sqrt{2}} (\Phi_{33}^{k(X_1)} \Psi_{36}^{k(X_1)} + \Phi_{36}^{k(X_1)} \Psi_{33}^{k(X_1)})$$

$$\Psi_{12}^{k(\Gamma_{5-})} = \frac{1}{\sqrt{2}} (\Phi_{22}^{k(X_1)} \Psi_{25}^{k(X_1)} + \Phi_{25}^{k(X_1)} \Psi_{22}^{k(X_1)})$$

$$\Psi_{13}^{k(\Gamma_{5-})} = \frac{1}{\sqrt{2}} (\Phi_{11}^{k(X_1)} \Psi_{14}^{k(X_1)} + \Phi_{14}^{k(X_1)} \Psi_{11}^{k(X_1)}).$$

For $X_1 \times X_1 = [M_{1-}]$ we have from table VIII of reference [30]

$$\Psi_{11}^{k(M_{1-})} = \frac{1}{\sqrt{2}} (\Phi_{11}^{k(X_1)} \Psi_{25}^{k(X_1)} + \Phi_{25}^{k(X_1)} \Psi_{11}^{k(X_1)}).$$

For $X_1 \times X_1 = M_{3-}$

$$\Psi_{11}^{k(M_{3-})} = \frac{1}{\sqrt{2}} (\Phi_{14}^{k(X_1)} \Psi_{22}^{k(X_1)} - \Phi_{22}^{k(X_1)} \Psi_{14}^{k(X_1)}).$$

For $M_{5+} \times M_{5+} = [\Gamma_{5+}] + \Gamma_{4+}$ from table V

$$\Psi_{11}^{k(\Gamma_{5+})} = \frac{1}{\sqrt{2}} (\Phi_{11}^{k(M_{5+})} \Psi_{14}^{k(M_{5+})} + \Phi_{14}^{k(M_{5+})} \Psi_{11}^{k(M_{5+})})$$

$$\Psi_{12}^{k(\Gamma_{5+})} = \frac{1}{\sqrt{2}} (\Phi_{33}^{k(M_{5+})} \Psi_{36}^{k(M_{5+})} + \Phi_{36}^{k(M_{5+})} \Psi_{33}^{k(M_{5+})})$$

$$\Psi_{13}^{k(\Gamma_{5+})} = \frac{1}{\sqrt{2}} (\Phi_{22}^{k(M_{5+})} \Psi_{25}^{k(M_{5+})} + \Phi_{25}^{k(M_{5+})} \Psi_{22}^{k(M_{5+})})$$

$$\Psi_{11}^{k(\Gamma_{4+})} = \frac{1}{\sqrt{2}} (\Phi_{11}^{k(M_{5+})} \Psi_{14}^{k(M_{5+})} - \Phi_{14}^{k(M_{5+})} \Psi_{11}^{k(M_{5+})})$$

$$\Psi_{12}^{k(\Gamma_{4+})} = \frac{1}{\sqrt{2}} (\Phi_{33}^{k(M_{5+})} \Psi_{36}^{k(M_{5+})} - \Phi_{36}^{k(M_{5+})} \Psi_{33}^{k(M_{5+})})$$

$$\Psi_{13}^{k(\Gamma_{4+})} = \frac{1}{\sqrt{2}} (\Phi_{22}^{k(M_{5+})} \Psi_{25}^{k(M_{5+})} - \Phi_{25}^{k(M_{5+})} \Psi_{22}^{k(M_{5+})}).$$

For $R_4 \times R_4 = \Gamma_{3-}$ from table XII of reference [30] we have

$$\Psi_{11}^{k(\Gamma_{3-})} = -\frac{1}{\sqrt{3}} (\Phi_{14}^{k(R_4)} \Psi_{11}^{k(R_4)} + \omega \Phi_{15}^{k(R_4)} \Psi_{13}^{k(R_4)} + \omega^2 \Phi_{16}^{k(R_4)} \Psi_{12}^{k(R_4)})$$

$$\Psi_{12}^{k(\Gamma_{3-})} = \frac{1}{\sqrt{3}} (\Phi_{11}^{k(R_4)} \Psi_{14}^{k(R_4)} + \omega \Phi_{12}^{k(R_4)} \Psi_{16}^{k(R_4)} + \omega^2 \Phi_{13}^{k(R_4)} \Psi_{15}^{k(R_4)}).$$

For $R_4 \times R_4 = \Gamma_4-$

$$\Psi_{11}^{\mathbf{k}(\Gamma_4-)} = \frac{1}{\sqrt{2}} (\Phi_{13}^{\mathbf{k}(R_4)} \Psi_{16}^{\mathbf{k}(R_4)} - \Phi_{16}^{\mathbf{k}(R_4)} \Psi_{13}^{\mathbf{k}(R_4)})$$

$$\Psi_{12}^{\mathbf{k}(\Gamma_4-)} = \frac{1}{\sqrt{2}} (\Phi_{11}^{\mathbf{k}(R_4)} \Psi_{15}^{\mathbf{k}(R_4)} - \Phi_{15}^{\mathbf{k}(R_4)} \Psi_{11}^{\mathbf{k}(R_4)})$$

$$\Psi_{13}^{\mathbf{k}(\Gamma_4-)} = \frac{1}{\sqrt{2}} (\Phi_{12}^{\mathbf{k}(R_4)} \Psi_{14}^{\mathbf{k}(R_4)} - \Phi_{14}^{\mathbf{k}(R_4)} \Psi_{12}^{\mathbf{k}(R_4)}) .$$

5. **Applications.** — In an effort to try to understand the properties of the superconducting compounds crystallizing in the A-15 structure much attention has been offered to the electronic bands and phonon modes at points of highest symmetry in the Brillouin zone. Gorkov *et al.* [8] proposed a theory based on the supposed proximity of the Fermi level to the $X_{1,2}$ electron bands at the X-point on the Brillouin zone boundary.

Achar and Barsch [14] developed a theory of the phonon dispersion relations for compounds with A-15 structure, in particular V_3Si and Nb_3Sn . The results exhibit the observed softening of the TA mode in [110], and of the LA mode in [100] direction, leading eventually to a lattice instability.

Jaric and Birman [36] analysed the polynomial invariants of the O_h^3 space group. Also they examined by group theoretical analysis possible lower symmetry phases arising from the A-15 structure [11].

Birman *et al.* [18] constructed the effective mass Hamiltonian at the X-point band edge, using the CG coefficients for O_h^3 deduced from those for O_h^7 . Ting-Kuo Lee *et al.* [37, 38] introduced a three-dimensional effective mass model for the electronic structure of A-15 compounds, based on the six-dimensional irreducible representation R_4 of the space group O_h^3 . By locating the Fermi Level near the maximum

of the density of states a free energy has been obtained which accounts quantitatively for normal state physical properties of the A-15 compounds. For the explicit construction of the effective Hamiltonian matrix the generalized $\mathbf{k}\cdot\mathbf{p}$ method was used, exploiting the method of invariants, first given by Luttinger [39] and elaborated by Bir and Pikus [40].

The construction can be performed by use of the CG coefficients and the symmetry adapted components of tensorial field quantities $\mathcal{K}_\alpha^{\mathbf{k}l}$. According to Birman *et al.* [18] the effective Hamiltonian matrix is

$$\mathcal{H}_{\alpha\alpha'}(\mathcal{K}) = \sum_{l''} a_{l''} \sum_{\alpha''} U^{-1\mathbf{k}(l) \times \mathbf{k}(l)}_{\alpha\alpha\alpha', \mathbf{k}''l''\gamma\sigma''\alpha''} \mathcal{K}_{\alpha''}^{\mathbf{k}''l''*} \quad (14)$$

Here the reduced matrix elements $a_{l''}$ are constants independent of α , α' and α'' .

The Clebsch-Gordan i.e. vector coupling coefficients by their definition enable one to obtain the correct symmetry adapted bilinear combinations of functions and thus permit one to make explicit use of symmetry of the problem.

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