CHAPTER III

EXPLICIT EXTRACTION OF PARAMETERS

The first step in the application of an interpolation scheme is the extraction of the values of the parameters. This may be done by fitting the interpolated bands at symmetry points with accurately calculated bands, and later, if desired, they may be changed in order to secure the best possible agreement with available experimental data. This fitting is feasible because, at certain points of high symmetry in the Brillouin zone, the Hamiltonian secular determinant can be quite readily diagonalized by the eigenvectors explicitly. The resultant expressions form groups with each group involving a closed set of the parameters. There are certain energy eigenvalues which are represented, even at points of symmetry, by expressions involving complicated arrays of the parameters. However, by proceeding in a judicious step-by-step, it turns out to be possible to extract all the 17 parameters employed in our scheme.

The eigenstates labelled by the symmetry notations Γ_{12}, $\Gamma_{25'}$, X_5, X_2, X_3, L_{31}, L_{32}, and K_4 are pure d levels and their eigenfunctions do not hybridize with the conduction bands. The explicit energy expressions for these levels involve only the 8 parameters, E_0, Δ, $A_1, \ldots, A_6$.

As there are 8 independent expressions for the 8 eigenvalues, the 8 adjustable parameters can be determined uniquely. The parameter β is fixed by the eigenvalue Γ_1 which is also taken as the zero of the energy scale. In the conduction bands, there are only three energy eigenvalues, labelled by Γ_1, $L_{2'}$, and $X_{4'}$, which are pure conduction eigenstates not hybridizing with the d levels. However, in our scheme, the $L_{2'}$ and $X_{4'}$ eigenvalues depend on the orthogonalization parameters K_o and R_o as well as the pseudopotential Fourier coefficients V_{111} and V_{200} and the parameter α. The extraction of these parameters, and the hybridization parameters K_2, K_3, and R_1 are more involved, as the simultaneous equations linking all these parameters are not linear. However, by trial and error, we have succeeded in finding the sequence of algebraic operations which permit the explicit extraction of all the parameters.

1 Pure d States

Consider first the pure d band eigenvalue $E(\Gamma_{25'})$. In the representation spanned by the following basis vectors:

$$
\begin{aligned}
\nu &= 1 & \varphi_{\vec{k}+\vec{K}_1} \\
\nu &= 2 & \varphi_{\vec{k}+\vec{K}_2} \\
\nu &= 3 & \varphi_{\vec{k}+\vec{K}_3} \\
\nu &= 4 & \varphi_{\vec{k}+\vec{K}_4} \\
\nu &= 5 & \varphi_{xy} \\
\nu &= 6 & \varphi_{yz} \\
\nu &= 7 & \varphi_{zx} \\
\nu &= 8 & \varphi_{x^2-y^2} \\
\nu &= 9 & \varphi_{3z^2-r^2}
\end{aligned}
\qquad (3.1)
$$

the eigenvector for the state with symmetry $\Gamma_{25'}$ is

$$e(\Gamma_{25'}) = \frac{1}{\sqrt{3}} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} . \tag{3.2}$$

The eigenvalue $E(\Gamma_{25'})$ is given by

$$E(\Gamma_{25'}) = \frac{1}{\sqrt{3}}\left[0\,0\,0\,0\,1\,1\,1\,0\,0\right] \begin{bmatrix} H_{11} & H_{12} & \cdots & H_{19} \\ H_{21} & H_{22} & \cdots & H_{29} \\ \vdots & & & \vdots \\ H_{91} & \cdots & \cdots & H_{99} \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \frac{1}{\sqrt{3}} \tag{3.3}$$

$$= \frac{1}{3}\left[0\,0\,0\,0\,1\,1\,1\,0\,0\right] \begin{pmatrix} H_{15} + H_{16} + H_{17} \\ H_{25} + H_{26} + H_{27} \\ \vdots \\ H_{95} + H_{96} + H_{97} \end{pmatrix}$$

$$= \frac{1}{3}\left[(H_{55}+H_{56}+H_{57}) + (H_{65}+H_{66}+H_{67}) + (H_{75}+H_{76}+H_{77})\right] . \tag{3.4}$$

At $\Gamma(0,0,0)$, the reduced coordinates ξ, η, and ζ in (2.30) have the values

$$\xi = 0 , \quad \eta = 0 , \quad \zeta = 0 . \tag{3.5}$$

Therefore, the values of the matrix elements, as shown in (2.29), are

$$\begin{aligned} H_{55} &= E_o - 4A_1 + 8A_2 , \\ H_{56} &= 0 , \\ H_{57} &= 0 , \\ H_{65} &= 0 , \\ H_{66} &= E_o - 4A_1 + 8A_2 , \\ H_{67} &= 0 , \\ H_{75} &= 0 , \\ H_{76} &= 0 , \\ H_{77} &= E_o - 4A_1 + 8A_2 . \end{aligned} \tag{3.6}$$

Substituting in (3.4), we obtain

$$E(\Gamma_{25'}) = E_o - 4A_1 + 8A_2 . \tag{3.7}$$

By performing the same type of operation, we obtain the 8 expressions for the 8 pure d levels as follows:

I $\quad E(\Gamma_{25'}) = E_o-4A_1+8A_2$

II $\quad E(\Gamma_{12}) = E_o+\Delta+4A_4-8A_5$

$$
\begin{array}{llcl}
\text{III} & E(X_5) & = & E_o+4A_1 \\
\text{IV} & E(X_3) & = & E_o-4A_1-8A_2 \\
\text{V} & E(X_2) & = & E_o+\Delta+4A_4+8A_5 \\
\text{VI} & E(K_4) & = & E_o+\Delta+2A_4+4\sqrt{2}A_5 \\
\text{VII} & E(L_{31}) & = & E_o+(\Delta)/2+2A_3-(1/2)\left[(\Delta-4A_3)^2+128A_6^2\right]^{\frac{1}{2}} \\
\text{VIII} & E(L_{32}) & = & E_o+(\Delta)/2+2A_3+(1/2)\left[(\Delta-4A_3)^2+128A_6^2\right]^{\frac{1}{2}}.
\end{array}
\qquad (3.8)
$$

The 8 parameters are extracted explicitly through the following sequence of equations:

$$
\begin{array}{llcl}
1. & A_2 & = & \frac{1}{16}\left[E(\Gamma_{25'})-E(X_3)\right] \\
2. & A_1 & = & \frac{1}{8}E(X_5)-\frac{1}{16}\left[E(\Gamma_{25'})+E(X_3)\right] \\
3. & E_o & = & \frac{1}{2}E(X_5)+\frac{1}{4}\left[E(\Gamma_{25'})+E(X_3)\right] \\
4. & A_5 & = & \frac{1}{16}\left[E(X_2)-E(\Gamma_{12})\right] \\
5. & A_4 & = & \frac{1}{2}\left[E(\Gamma_{12})-E(K_4)\right]+2(2+\sqrt{2})A_5 \\
6. & \Delta & = & E(\Gamma_{12})+8A_5-E_o-4A_4 \\
7. & A_3 & = & \frac{1}{4}\left[E(L_{31})+E(L_{32})\right]-\frac{1}{2}E_o-\frac{1}{4}\Delta
\end{array}
\qquad (3.9)
$$

8. Solve for A_6 from

$$E(L_{31})+E(L_{32}) = \left[(\Delta-4A_3)^2+128A_6^2\right]^{\frac{1}{2}} .$$

2 Pure Conduction States

As the algebraic expressions get more involved, there is a need to introduce progessive abbreviations. Eventually, the computer has to be employed. For simplicity, we, therefore, introduce the following notations:

$$
\begin{aligned}
K_o &= B_5 , \\
R_o &= B_4 , \\
K_3 &= B_3 , \\
K_2 &= B_2 , \\
R_1 &= B_1 , \\
V_{111} &= V_1 , \\
V_{200} &= V_2 .
\end{aligned}
\qquad (3.10)
$$

From now on, the 17 parameters in our scheme are denoted by

$$
\begin{aligned}
&E , \quad \Delta, \quad A_1, \quad A_2, \quad A_3, \quad A_4, \quad A_5, \quad A_6, \\
&\alpha , \quad \beta, \quad V_1, \quad V_2, \quad B_1, \quad B_2, \quad B_3, \quad B_4, \quad B_5.
\end{aligned}
\qquad (3.11)
$$

There are three pure conduction band states which we shall concern with. They are labelled by the symmetry notations Γ_1, $X_{4'}$, and $L_{2'}$. Their properly symmetrized eigenfunctions, in our representation, are the following (see Appendix A):

$$
\begin{array}{lcl}
\nu & : & 1\ 2\ 3\ 4\ 5\ 6\ 7\ 8\ 9 \\
e(\Gamma_1) & = & [1\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0] \\
e(X_{4'}) & = & [1\ -1\ 0\ 0\ 0\ 0\ 0\ 0\ 0]\ (1/\sqrt{2}) \\
e(L_{2'}) & = & [1\ 0\ -1\ 0\ 0\ 0\ 0\ 0\ 0]\ (1/\sqrt{2})
\end{array}
\qquad (3.12)
$$

To calculate the pure conduction eigenvalues at these symmetry points, the above symmetrized eigenfunctions and the full 9x9 band Hamiltonian are used. Then

$$E(\Gamma_1) = e^T(\Gamma_1) H e(\Gamma_1)$$

giving

$$E(\Gamma_1) = H_{11} \quad . \qquad (3.13)$$

Similarly, we obtain

$$E(X_{4'}) = \frac{1}{2}(H_{11}-H_{12}-H_{21}+H_{22}) \qquad (3.14)$$

and

$$E(L_{2'}) = \frac{1}{2}(H_{11}-H_{13}-H_{31}+H_{33}) \quad . \qquad (3.15)$$

At Γ : $\vec{k}^{\Gamma} = (0,0,0)$, $k^{\Gamma} = |\vec{k}^{\Gamma}| = 0$.

Since $j_2(0) = 0$,

$f(k^{\Gamma}) = 0$, $g(k^{\Gamma}) = 0$,

and $C_{\vec{k}^{\Gamma}} = 1$.

As $H_{11}^{IV} = 0$, $H_{11}^{V} = 0$, and $H_{11}^{I} = \beta$,

we have $H_{11} = \beta$.

Therefore $E(\Gamma_1) = \beta$.

In other word, the value of β is simply fixed at the bottom of the conduction band $E(\Gamma_1)$.

In the evaluation of the matrix elements of the OPW-OPW block, as given in (2.43)-(2.47), and the OPW-LCAO block, as given in (2.56), we often require the values of the products $C_n F_n(\vec{k}_i)$. We therefore tabulate here the values of these products at the various symmetry points. All wave-vectors and reciprocal lattice vectors are expressed in units of $\frac{\pi}{4a}$ (a : lattice constant) .

At X : $\vec{k}^X = (0,8,0)$, $k^X = |\vec{k}^X| = 8$.

$$\begin{aligned} \vec{k}_1^X &= \vec{k}^X + \vec{K}_1 = (0,8,0) , & k_1^X &= 8 = k^X , \\ \vec{k}_2^X &= \vec{k}^X + \vec{K}_2 = (0,-8,0) , & k_2^X &= 8 = k^X , \\ \vec{k}_3^X &= \vec{k}^X + \vec{K}_3 = (-8,0,-8) , & k_3^X &= 8\sqrt{2} , \\ \vec{k}_4^X &= \vec{k}^X + \vec{K}_4 = (-8,0,8) , & k_4^X &= 8\sqrt{2} . \end{aligned} \qquad (3.16)$$

Values of $C_n F_n(\vec{k}_i^X)$

i \ n	5	6	7	8	9
1	0	0	0	$-\frac{1}{2}$	$-\frac{1}{2\sqrt{3}}$
2	0	0	0	$-\frac{1}{2}$	$-\frac{1}{2\sqrt{3}}$
3	0	0	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4\sqrt{3}}$
4	0	0	$-\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4\sqrt{3}}$

(3.17)

At L : $\vec{k}^L = (4,4,4)$, $k^L = |\vec{k}^L| = \sqrt{48}$.

$$
\begin{aligned}
\vec{k}^L_1 &= \vec{k}^L + \vec{K}_1 = (4,4,4) , & k^L_1 &= \sqrt{48} = k^L , \\
\vec{k}^L_2 &= \vec{k}^L + \vec{K}_2 = (4,-12,4) , & k^L_2 &= 4\sqrt{11} , \\
\vec{k}^L_3 &= \vec{k}^L + \vec{K}_3 = (-4,-4,-4) , & k^L_3 &= \sqrt{48} = k^L , \\
\vec{k}^L_4 &= \vec{k}^L + \vec{K}_4 = (-4,-4,-12) , & k^L_4 &= 4\sqrt{11} .
\end{aligned}
\qquad (3.18)
$$

<u>Values of $C_n F_n(\vec{k}^L_i)$</u>

i \ n	5	6	7	8	9
1	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0
2	$-\frac{3}{11}$	$-\frac{3}{11}$	$\frac{1}{11}$	$-\frac{4}{11}$	$\frac{4}{33}\sqrt{3}$
3	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0
4	$\frac{1}{11}$	$-\frac{3}{11}$	$-\frac{3}{11}$	0	$\frac{8}{33}\sqrt{3}$

(3.19)

At W : $\vec{k}^W = (4,8,0)$, $k^W = |\vec{k}^W| = \sqrt{80}$.

$$
\begin{aligned}
\vec{k}^W_1 &= \vec{k}^W + \vec{K}_1 = (4,8,0) , & k^W_1 &= \sqrt{80} = k^W , \\
\vec{k}^W_2 &= \vec{k}^W + \vec{K}_2 = (4,-8,0) , & k^W_2 &= \sqrt{80} = k^W , \\
\vec{k}^W_3 &= \vec{k}^W + \vec{K}_3 = (-4,0,-8) , & k^W_3 &= \sqrt{80} = k^W , \\
\vec{k}^W_4 &= \vec{k}^W + \vec{K}_4 = (-4,0,8) , & k^W_4 &= \sqrt{80} = k^W .
\end{aligned}
\qquad (3.20)
$$

Values of $C_nF_n(\vec{k}^W)$

i \ n	5	6	7	8	9
1	$\frac{2}{5}$	0	0	$-\frac{3}{10}$	$-\frac{1}{2\sqrt{3}}$
2	$-\frac{2}{5}$	0	0	$-\frac{3}{10}$	$-\frac{1}{2\sqrt{3}}$
3	0	0	$\frac{2}{5}$	$\frac{1}{10}$	$\frac{7}{10}\sqrt{3}$
4	0	0	$-\frac{2}{5}$	$\frac{1}{10}$	$\frac{7}{10}\sqrt{3}$

(3.21)

These tabulations have been checked by the relation (2.8)

$$\sum_n \left| C_nF_n(\vec{k}) \right|^2 = \frac{1}{3} \quad .$$

The orthogonalization form factor (2.43), hybridization form factor (2.44), and the normalization constants (2.49) at various symmetry points are listed below :

$$f_X = f(k^X) = B_5 j_2(k^X B_4) \ , \quad g_X = g(k^X) = B_3 j_2(k^X B_1) \ ,$$
$$C_X^2 = \left| C_{\vec{k}X} \right|^2 = 1 - \frac{1}{3} f_X^2 \ , \qquad (3.22)$$

$$f_L = f(k^L) = B_5 j_2(k^L B_4) \ , \quad g_L = g(k^L) = B_2 j_2(k^L B_1) \ ,$$
$$C_L^2 = \left| C_{\vec{k}L} \right|^2 = 1 - \frac{1}{3} f_L^2 \ , \qquad (3.23)$$

$$f_W = f(k^W) = B_5 j_2(k^W B_4) \ , \quad g_W = g(k^W) = B_3 j_2(k^W B_1) \ ,$$
$$C_W^2 = \left| C_{\vec{k}W} \right|^2 = 1 - \frac{1}{3} f_W^2 \quad . \qquad (3.24)$$

Then from (2.45) to (2.49) we have :

at X :

$$H^{I}_{11} = 64\alpha + \beta \;, \qquad H^{I}_{22} = H^{I}_{11} \;, \qquad H^{I}_{12} = V_2 \;,$$
$$H^{V}_{11} = -\tfrac{2}{3}\, C_X f_X g_X \;, \qquad H^{V}_{22} = H^{V}_{11} \;, \qquad H^{V}_{12} = H^{V}_{11} \;, \tag{3.25}$$

$$\begin{aligned} H^{IV}_{11} &= \left[\left(-\tfrac{1}{2}\right)^2 f_X^2\, H_{88} + \left(-\tfrac{1}{2\sqrt{3}}\right)^2 f_X^2\, H_{99} + 2\left(-\tfrac{1}{2}\right)\left(\tfrac{-1}{2\sqrt{3}}\right) f_X^2\, H_{89}\right] \\ &= \tfrac{1}{4} f_X^2 \left[H_{88} + \tfrac{1}{3} H_{99} + \tfrac{2}{\sqrt{3}} H_{89} \right] \\ &= \tfrac{1}{3} f_X^2 \left[E_o + \Delta - \tfrac{20}{3} A_4 - \tfrac{8}{3} A_5 \right] \;. \end{aligned} \tag{3.26}$$

If the eigenstates X_1 had been an unhybridized level, and if we follow the steps leading to (3.7), we will obtain the d-contribution to the eigenvalue of X_1 as

$$E^d(X_1) = E_o + \Delta - \tfrac{20}{3} A_4 - \tfrac{8}{3} A_5 \;. \tag{3.27}$$

Then (3.26) becomes

$$H^{IV}_{11} = \tfrac{1}{4} f_X^2\, E^d(X_1) \;. \tag{3.28}$$

Similarly, we have

$$H^{IV}_{22} = H^{V}_{11} \;, \qquad H^{IV}_{12} = H^{IV}_{11} \;. \tag{3.29}$$

Combining (3.25), (3.28), and (3.29) according to (2.45), we have

$$\begin{aligned} H_{11} = H_{22} &= C_X^{-2} \left[64\alpha + \beta - \tfrac{2}{3} C_X f_X g_X - \tfrac{1}{3} f_X^2\, E^d(X_1) \right] \\ H_{12} &= C_X^{-2} \left[V_2 - \tfrac{2}{3} C_X f_X g_X - \tfrac{1}{3} f_X^2\, E^d(X_1) \right] \;. \end{aligned} \tag{3.30}$$

Therefore Eq.(3.14) gives

$$E(X_{4'}) = C_X^{-2}\left(\beta + 64\alpha - V_2\right) \tag{3.31}$$

with C_X^{-2} given by (3.22); namely

$$C_X^{-2} = \left(1 - \frac{1}{3} f_X^2\right)^{-1} = \left[1 - \frac{1}{3} B_5^2 j_2^2(k^X B_4)\right]^{-1} .$$

Similarly, we have, at L ,

$$\begin{aligned} H_{11}^{I} &= 48\alpha + \beta , & H_{33}^{I} &= H_{11}^{I} , & H_{13}^{I} &= V_1 , \\ H_{11}^{V} &= -\frac{2}{3} C_L f_L g_L , & H_{33}^{V} &= H_{11}^{V} , & H_{13}^{V} &= H_{11}^{V} , \\ H_{13}^{IV} &= -\frac{1}{3} f_L^2 E^d(L_1), & H_{33}^{IV} &= H_{11}^{IV} , & H_{13}^{IV} &= H_{11}^{IV} , \end{aligned} \tag{3.32}$$

with

$$E^d(L_1) = E_o - 8A_3 . \tag{3.33}$$

Therefore

$$H_{11} = H_{33} = C_L^{-2}\left[48\alpha + \beta - \frac{2}{3} C_L f_L g_L - \frac{1}{3} f_L^2 E^d(L_1)\right] . \tag{3.34}$$

$$H_{13} = C_L^{-2}\left[V_1 - \frac{2}{3} C_L f_L g_L - \frac{1}{3} f_L^2 E^d(L_1)\right] . \tag{3.35}$$

Then (3.15) gives

$$E(L_{2'}) = C_L^{-2}\left[\beta + 48\alpha - V_1\right] \tag{3.36}$$

with C_L^{-2} given by Eq.(3.23); namely

$$C_L^{-2} = \left(1 - \frac{1}{3} f_L^2\right)^{-1} = \left[1 - \frac{1}{3} B_5^2 j_2^2(k^L B_4)\right]^{-1} .$$

It is useful to summarize at this point the unhybridized levels :

Pure d levels

$$\begin{array}{llll}
\text{I} & E(\Gamma_{25'}) & = & E_o-4A_1+8A_2 \\
\text{II} & E(\Gamma_{12}) & = & E_o+\Delta+4A_4-8A_5 \\
\text{III} & E(X_5) & = & E_o+4A_1 \\
\text{IV} & E(X_3) & = & E_o-4A_1-8A_2 \\
\text{V} & E(X_2) & = & E_o+\Delta+4A_4+8A_5 \\
\text{VI} & E(K_4) & = & E_o+\Delta+2A_4+4\sqrt{2}A_5 \\
\text{VII} & E(L_{31}) & = & E_o+(\Delta/2)+2A_3-(1/2)\left[(\Delta-4A_3)^2+128A_6^2\right]^{\frac{1}{2}} \\
\text{VIII} & E(L_{32}) & = & E_o+(\Delta/2)+2A_3+(1/2)\left[(\Delta-4A_3)^2+128A_6^2\right]^{\frac{1}{2}}
\end{array} \qquad (3.37)$$

Pure conduction levels

$$\begin{array}{llll}
\text{IX} & E(\Gamma_1) & = & \beta \\
\text{X} & E(X_{4'}) & = & C_X^{-2}\left[\beta+64\alpha-V_2\right] \\
 & & = & \left[1-\frac{1}{3}B_5^2j_2^2(k^XB_4)\right]^{-1}\left[\beta+64\alpha-V_2\right] \\
\text{XI} & E(L_{2'}) & = & C_L^{-2}\left[\beta+48\alpha-V_1\right] \\
 & & = & \left[1-\frac{1}{3}B_5^2j_2^2(k^LB_4)\right]^{-1}\left[\beta+48\alpha-V_1\right]
\end{array} \qquad (3.38)$$

For the first group of pure d levels, eight parameters are related by eight independent simultaneous equations, and the eight parameters can be solved without much trouble, as indicated in Eqs.(3.9) .

For the second group, the first equation determines β uniquely. The remaining two equations involving 5 parameters yet to be determined; namely α, V_1, V_2, B_4, and B_5. There are three more parameters to be determined, those signifying hybridization effects : B_1, B_2, B_3 . For these 8 parameters, at least 6 more independent relations are required to determine all parameters uniquely. These are sought for from the hybridized states.

3 Hybridized States

In the range of energy under consideration, there are 3 other eigenvalues available from accurate first-principles calculations which are not yet utilized in the fitting process; namely, X_1, L_1, and $W_{2'}$. These are the hybridized states. In our notation, their eigenvectors are :

$$e(X_1) = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\ \frac{1}{\sqrt{2}}\ 0\ 0\ 0\ 0\ 0\ \frac{\sqrt{3}}{2}\ \frac{1}{2}\right), \quad (3.39)$$

$$e(L_1) = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\ 0\ \frac{1}{\sqrt{2}}\ 0\ \frac{1}{\sqrt{3}}\ \frac{1}{\sqrt{3}}\ \frac{1}{\sqrt{3}}\ 0\ 0\right), \quad (3.40)$$

$$e(W_{2'}) = \frac{1}{\sqrt{2}}\left(\frac{1}{2}\ \frac{1}{2}\ -\frac{1}{2}\ -\frac{1}{2}\ 0\ 0\ 0\ \frac{1}{2}\ \frac{\sqrt{3}}{2}\right). \quad (3.41)$$

Again expressing the eigenvalues in terms of the Hamiltonian matrix elements through

$$E(X_1) = e^{\dagger}(X_1)He(X_1) \quad , \text{ etc.,}$$

we have

$$E(X_1) = \frac{1}{4}[H_{11}+H_{22}+2H_{12}+\frac{1}{2}(3H_{88}+H_{99})+\sqrt{3}H_{89} +\sqrt{6}(H_{18}+H_{28})+\sqrt{2}(H_{19}+H_{29})] \quad (3.42)$$

$$E(L_1) = \frac{1}{12}[3(H_{11}+H_{33}+2H_{13})+2(H_{55}+H_{66}+H_{77}+2H_{56} +2H_{57}+2H_{67})+2\sqrt{6}(H_{15}+H_{16}+H_{17}+H_{35}+H_{36}+H_{37})] \quad (3.43)$$

$$E(W_{2'}) = \frac{1}{8}[H_{11}+H_{22}+H_{33}+H_{44}+2(H_{12}-H_{13}-H_{14}-H_{23}-H_{24}+H_{34})+H_{88}+3H_{99}+2\sqrt{3}H_{89}+2(H_{18}+H_{28}-H_{38}-H_{48})+2\sqrt{3}(H_{19}+H_{29}-H_{39}-H_{49})] \quad (3.44)$$

The matrix elements for the OPW-OPW block ($H_{\nu\nu'}$; $\nu, \nu' \leq 4$) for the symmetry points X and L have been calculated in (3.30), (3.34) and (3.35). The matrix elements for the symmetry point W can be calculated in the same way, although through a somewhat lengthier procedure. These matrix elements are listed below :

X :
$$H_{11} = H_{22} = C_X^{-2}[\beta+64\alpha-\tfrac{2}{3}C_X f_X g_X-\tfrac{1}{3}f_X^2 E^d(X_1)]$$
$$H_{12} = C_X^{-2}[V_2-\tfrac{2}{3}C_X f_X g_X-\tfrac{1}{3}f_X^2 E^d(X_1)] \quad (3.30)$$

L :
$$H_{11} = H_{33} = C_L^{-2}[\beta+48\alpha-\tfrac{2}{3}C_L f_L g_L-\tfrac{1}{3}f_L^2 E^d(L_1)] \quad (3.34)$$
$$H_{13} = C_L^{-2}[V_1-\tfrac{2}{3}C_L f_L g_L-\tfrac{1}{3}f_L^2 E^d(L_1)] \quad (3.35)$$

W :
$$H_{11} = H_{22} = H_{33} = H_{44} = C_W^{-2}[\beta+80\alpha-\tfrac{2}{3}C_W f_W g_W-\tfrac{1}{75}f_W^2\{E^d(W_1)+12E^d(W_{2'})+12E^d(W_3)\}] \quad (3.45)$$
$$H_{12} = H_{34} = C_W^{-2}[V_2-\tfrac{2}{75}C_W f_W g_W-\tfrac{1}{75}f_W^2\{E^d(W_1)+12E^d(W_{2'})-12E^d(W_3)\}] \quad (3.46)$$
$$H_{13} = H_{14} = H_{23} = H_{24} = C_W^{-2}[V_1+\tfrac{22}{75}C_W f_W g_W-\tfrac{1}{75}f_W^2\{E^d(W_1)-12E^d(W_{2'})\}] \quad (3.47)$$

The symbols C_X^2, C_L^2, C_W^2, f_X, f_L, f_W, g_X, g_L, g_W were defined in (3.22)—(3.24). Notations like $E^d(X_1)$ represent the d-electron contribution to energy of the state of that symmetry and could be calculated in the same way as the derivation of (3.8). Their values in terms of our parameters are listed below :

$$E^d(X_1) = E_o + \Delta - \frac{20}{3}A_4 - \frac{8}{3}A_5 \qquad (3.48)$$

$$E^d(L_1) = E_o - 8A_3 \qquad (3.49)$$

$$E^d(W_1) = E_o + \Delta + \frac{4}{3}A_4 + \frac{16}{3}A_5 \qquad (3.50)$$

$$E^d(W_{2'}) = E_o + \Delta - 4A_4 \qquad (3.51)$$

$$E^d(W_3) = E_o - 4A_2 \qquad (3.52)$$

The matrix elements of the LCAO-LCAO block ($H_{\nu\nu'}$; $5 \leq \nu, \nu' \leq 9$) at the symmetry points X, L, W are easily written down from the general expressions given in (2.29) :

X : $\vec{k}^X = \frac{2\pi}{a}(0,1,0) = \frac{\pi}{4a}(0,8,0)$: $\xi = 0$, $\eta = \pi$, $\zeta = 0$:

$$\begin{aligned} H_{55} = H_{66} &= E_o + 4A_1 \\ H_{77} &= E_o - 4A_1 - 8A_2 \\ H_{88} &= E_o + \Delta - 4A_4 \\ H_{99} &= E_o + \Delta + \frac{4}{3}A_4 + \frac{16}{3}A_5 \\ H_{56} = H_{57} = H_{58} = H_{59} = H_{67} = H_{68} = H_{69} = H_{78} = H_{79} &= 0 \\ H_{89} &= -\frac{8}{\sqrt{3}}A_4 - \frac{8}{\sqrt{3}}A_5 \end{aligned} \qquad (3.53)$$

$$L: \quad \vec{k}^L = \frac{2\pi}{a}\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right) = \frac{\pi}{4a}(4,4,4): \quad \xi = \frac{\pi}{2}, \quad \eta = \frac{\pi}{2}, \quad \zeta = \frac{\pi}{2}:$$

$$\begin{aligned}
H_{55} = H_{66} = H_{77} &= E_o \\
H_{88} = H_{99} &= E_o + \Delta \\
H_{56} = H_{57} = H_{67} &= -4A_3 \\
H_{58} = H_{89} &= 0 \\
H_{59} &= -\frac{8}{\sqrt{3}}A_6 \\
H_{68} = -H_{78} &= -4A_6 \\
H_{69} = H_{79} &= \frac{4}{\sqrt{3}}A_6
\end{aligned} \qquad (3.54)$$

$$W: \quad \vec{k}^W = \frac{2\pi}{a}\left(\frac{1}{2},1,0\right) = \frac{\pi}{4a}(4,8,0): \quad \xi = \frac{\pi}{2}, \quad \eta = \pi, \quad \zeta = 0:$$

$$\begin{aligned}
H_{55} = H_{77} &= E_o - 4A_2 \\
H_{66} &= E_o + 4A_1 \\
H_{88} &= E_o + \Delta + 4A_5 \\
H_{99} &= E_o + \Delta - \frac{8}{3}A_4 + \frac{4}{3}A_5 \\
H_{56} = H_{57} = H_{58} = H_{59} = H_{67} = H_{68} = H_{69} = H_{78} = H_{79} &= 0 \\
H_{89} &= -\frac{4}{\sqrt{3}}A_4 - \frac{4}{\sqrt{3}}A_5
\end{aligned} \qquad (3.55)$$

The matrix elements of the OPW-LCAO block ($H_{\nu\nu'}$; $\nu \leq 4$, $5 \leq \nu' \leq 9$) for the symmetry points X, L, W are easily written down from (2.56) and are listed below :

$$X: \quad \begin{aligned}
H_{18} = H_{28} &= -\frac{1}{2}g_X \\
H_{19} = H_{29} &= -\frac{1}{2\sqrt{3}}g_X
\end{aligned} \qquad (3.56)$$

$$L: \quad H_{15} = H_{16} = H_{17} = \frac{1}{3}g_L \qquad (3.57)$$
$$H_{35} = H_{36} = H_{37} = \frac{1}{3}g_L$$

$$W: \quad H_{15} = \frac{2}{5}g_W, \; H_{25} = -\frac{2}{5}g_W, \; H_{35} = 0, \; H_{45} = 0,$$
$$H_{17} = 0, \; H_{27} = 0, \; H_{37} = \frac{2}{5}g_W, \; H_{48} = -\frac{2}{5}g_W,$$
$$H_{18} = -\frac{3}{10}g_W, \; H_{28} = -\frac{3}{10}g_W, \; H_{38} = \frac{1}{10}g_W, \; H_{48} = \frac{1}{10}g_W,$$
$$H_{19} = -\frac{1}{2\sqrt{3}}g_W, \; H_{29} = -\frac{1}{2\sqrt{3}}g_W, \; H_{39} = \frac{7}{10\sqrt{3}}g_W, \; H_{49} = \frac{7}{10\sqrt{3}}g_W. \qquad (3.58)$$

where $g_X = B_3 j_2(k^X R_1)$, $g_L = B_2 j_2(k^L R_1)$, (3.59)

and $g_W = B_3 j_2(k^W R_1)$.

Substituting the values of the matrix elements into (3.42)—(3.44), we get the resultant expressions for the states with symmetry X_1, L_1 and $W_{2'}$ respectively as follows :

$$E(X_1) = \frac{1}{2}[E^s(X_1)+E^d(X_1)] + \gamma(X_1), \qquad (3.60)$$
$$E(L_1) = \frac{1}{2}[E^s(L_1)+E^d(L_1)] + \gamma(L_1), \qquad (3.61)$$
$$E(W_{2'}) = \frac{1}{2}[E^s(W_{2'})+E^d(W_{2'})] + \gamma(W_{2'}), \qquad (3.62)$$

where

$$E^s(X_1) = C_X^{-2}[\beta + 64\alpha + V_2 - \frac{4}{3}C_X f_X g_X - \frac{2}{3}f_X^2 E^d(X_1)] \qquad (3.63)$$
$$E^s(L_1) = C_L^{-2}[\beta + 48\alpha + V_1 - \frac{4}{3}C_L f_L g_L - \frac{2}{3}f_L^2 E^d(L_1)] \qquad (3.64)$$
$$E^s(W_{2'}) = C_W^{-2}[\beta + 80\alpha + V_2 - 2V_1 - \frac{32}{75}C_W f_W g_W - \frac{16}{25}f_W^2 E^d(W_{2'})] \qquad (3.65)$$

are the energies of conduction bands with the designated symmetry if there were no hybridization,

$$E^d(X_1) = E_o + \Delta - \frac{20}{3}A_4 - \frac{8}{3}A_5$$

$$E^d(L_1) = E_o - 8A_3$$

$$E^d(W_{2'}) = E_o + \Delta - 4A_4$$

are the energies of d-bands with the designated symmetry if there were no hybridization, as given in (3.48)—(3.50), and

$$\gamma(X_1) = -\sqrt{\frac{2}{3}}\, g_X = -\sqrt{\frac{2}{3}}\, B_3 j_2(k^X B_1) \quad , \qquad (3.66)$$

$$\gamma(L_1) = \sqrt{\frac{2}{3}}\, g_L = \sqrt{\frac{2}{3}}\, B_2 j_2(k^L B_1) \quad , \qquad (3.67)$$

$$\gamma(W_{2'}) = -\frac{4}{5}\, g_W = -\frac{4}{5}\, B_3 j_2(k^W B_1) \quad . \qquad (3.68)$$

In a simplified notation it may be noted that when a conduction band of energy E^s and a d-band of energy E^d hybridize, the energies after hybridization may be obtained from solving the secular determinant :

$$\begin{vmatrix} E^s - E & \gamma \\ \gamma & E^d - E \end{vmatrix} = 0 \qquad (3.69)$$

where γ denotes the hybridization matrix element. This secular equation gives the energies :

$$E = \frac{1}{2}(E^s + E^d) \pm \frac{1}{2}\sqrt{(E^s - E^d)^2 + 4\gamma^2} \quad . \qquad (3.70)$$

It may be noted that where the two unhybridized levels cross (i.e., $E^s = E^d$), the energies are

$$E = \frac{1}{2}(E^s + E^d) \pm \gamma \tag{3.71}$$

Comparing with (3.60)—(3.62), we see that $\gamma(X_1)$, $\gamma(L_1)$, $\gamma(W_{2'})$ in (3.66)—(3.68) may be taken as the hybridization matrix elements for the states with the designated symmetries.

We will therefore take as expressions of the pair of hybridized states the following :

XII $$E(X_{11}) = \frac{1}{2}[E^s(X_1)+E^d(X_1)] - \frac{1}{2}[\{E^s(X_1)-E^d(X_1)\}^2+4\gamma^2(X_1)]^{\frac{1}{2}} \tag{3.72}$$

XIII $$E(X_{12}) = \frac{1}{2}[E^s(X_1)+E^d(X_1)] + \frac{1}{2}[\{E^s(X_1)-E^d(X_1)\}^2+4\gamma^2(X_1)]^{\frac{1}{2}} \tag{3.73}$$

XIV $$E(L_{11}) = \frac{1}{2}[E^s(L_1)+E^d(L_1)] - \frac{1}{2}[\{E^s(L_1)-E^d(L_1)\}^2+4\gamma^2(L_1)]^{\frac{1}{2}} \tag{3.74}$$

XV $$E(L_{12}) = \frac{1}{2}[E^s(L_1)+E^d(L_1)] + \frac{1}{2}[\{E^s(L_1)-E^d(L_1)\}^2+4\gamma^2(L_1)]^{\frac{1}{2}} \tag{3.75}$$

XVI $$E(W_{2',1}) = \frac{1}{2}[E^s(W_{2'})+E^d(W_{2'})] - \frac{1}{2}[\{E^s(W_{2'})-E^d(W_{2'})\}^2+4\gamma^2(W_{2'})]^{\frac{1}{2}} \tag{3.76}$$

XVII $$E(W_{2',2}) = \frac{1}{2}[E^s(W_{2'})+E^d(W_{2'})] + \frac{1}{2}[\{E^s(W_{2'})-E^d(W_{2'})\}^2+4\gamma^2(W_{2'})]^{\frac{1}{2}} \tag{3.77}$$

These equations, together with the eleven earlier listed as (3.37) and (3.38) are the 17 equations linking the 17 parameters. They are the 17 equations from which the 17 parameters are to be ultimately determined.

4 Algebraic Solution for the Parameters

To summarize the situation, we have 17 parameters to be fitted from 17 independent relations linking 17 first-principles calculated energy eigenvalues with 17 parameters. The first 8 of these relations, Nos. I-VIII, involve only 8 parameters; namely $E_0, \Delta, A_1, \ldots, A_6$. These parameters are already explicitly extracted in Eq.(3.9). Relation number IX determined the ninth parameter, β, directly. We are thus left with 8 independent relations; namely Nos. X-XVII, for the determination of the remaining 8 parameters; namely α, V_1, V_2, B_1, B_2, B_3, B_4, B_5. The parameter α is simply evaluated because its value depends only on the lattice constant, Eq.(2.35). There are eventually only 7 parameters to be extracted. These parameters will be extracted in the sequence B_1, B_2, B_3, B_4, B_5, V_1, V_2.

The most important step in the scheme for explicit extraction by the observation that isolation of the first single parameter; namely B_1, is possible through the following manipulation of the relations:

$$E(X_{11})+E(X_{12}) = E^s(X_1)+E^d(X_1) \quad , \quad (3.78)$$

$$E(W_{2,1})+E(W_{2,2}) = E^s(W_{2,})+E^d(W_{2,}) \quad , \quad (3.79)$$

$$\{E(X_{12})-E(X_{11})\}^2 = \{E^s(X_1)-E^d(X_1)\} +4\gamma^2(X_1) \quad , \quad (3.80)$$

$$\{E(W_{2,2})-E(W_{2,1})\}^2 = \{E^s(W_{2,})-E^d(W_{2,})\} +4\gamma^2(W_{2,}) \; . \quad (3.81)$$

Eliminating $E^s(X_1)$ and $E^s(W_{2'})$, we get

$$\begin{aligned}4\gamma^2(X_1) &= \{E(X_{12})-E(X_{11})\}^2-\{E(X_{11})+E(X_{12})-2E^d(X_1)\}^2\\ &= \{E(X_{12})-E(X_{11})-E(X_{11})-E(X_{12})+2E^d(X_1)\}\\ &\quad\times\{E(X_{12})-E(X_{11})+E(X_{11})+E(X_{12})-2E^d(X_1)\}\\ &= 4\{E^d(X_1)-E(X_{11})\}\{E(X_{12})-E^d(X_1)\}\ , \qquad (3.82)\end{aligned}$$

and

$$4\gamma^2(W_{2'}) = 4\{E^d(W_{2'})-E(W_{2'1})\}\{E(W_{2'2})-E^d(W_{2'})\}\ . \qquad (3.83)$$

Similarly, we can obtain

$$4\gamma^2(L_1) = 4\{E^d(L_1)-E(L_{11})\}\{E(L_{12})-E^d(L_1)\}\ . \qquad (3.84)$$

Taking the ratio of (3.82) and (3.83), we get

$$\frac{4\gamma^2(X_1)}{4\gamma^2(W_{2'})} = \frac{\left(-\sqrt{\frac{3}{3}}\right)^2 B_3^2\dot{\gamma}_2^2(k^X B_1)}{\left(-\frac{4}{5}\right)^2 B_3^2\dot{\gamma}_2^2(k^W B_1)} = \frac{25}{24}\times\frac{\dot{\gamma}_2^2(k^X B_1)}{\dot{\gamma}_2^2(k^W B_1)}$$

$$= \frac{\{E^d(X_1)-E(X_{11})\}\{E(X_{12})-E^d(X_1)\}}{\{E^d(W_{2'})-E(W_{2'1})\}\{E(W_{2'2})-E^d(W_{2'})\}}$$

yielding

$$\frac{\dot{\gamma}_2(k^X B_1)}{\dot{\gamma}_2(k^W B_1)} = \sqrt{\frac{24}{25}}\times\sqrt{\frac{\{E^d(X_1)-E(X_{11})\}\{E(X_{12})-E^d(X_1)\}}{\{E^d(W_{2'})-E(W_{2'1})\}\{E(W_{2'2})-E^d(W_{2'})\}}}\ . \qquad (3.85)$$

Iterating on a computer, the numerical value of B_1 can be extracted. With B_1 determined, Eq.(3.84) can be used to obtain B_2 :

$$B_2 = \sqrt{\frac{3}{2}}\times\sqrt{\{E^d(L_1)-E(L_{11})\}\{E(L_{12})-E^d(L_1)\}}\Big/\dot{\gamma}_2(k^L B_1)\ , \qquad (3.86)$$

and Eq.(3.82) can be used to obtain B_3 :

$$B_3 = \sqrt{\frac{3}{2}} \times \sqrt{\{E^d(X_1)-E(X_{11})\}\{E(X_{12})-E^d(X_1)\}} \Big/ j_2(k^X B_1) \quad . \quad (3.87)$$

The parameters B_4 and B_5 appearing in the orthogonality form factor can be extracted in a similar way. We now again introduce some simplifying notations :

$$X = E(X_{11})+E(X_{12})+E(X_{4'}) \quad , \quad (3.88)$$

$$L = E(L_{11})+E(L_{12})+E(L_{2'}) \quad . \quad (3.89)$$

Using Eqs. (3.72) and (3.73), we obtain

$$X = E^s(X_1)+E^d(X_1)+E(X_{4'}) \quad , \quad (3.90)$$

$$L = E^s(L_1)+E^d(L_1)+E(L_{2'}) \quad . \quad (3.91)$$

Substituting $E^s(X_1)$ as given in (3.63) and $E(X_{4'})$ as given in (3.31) into (3.90), we obtain

$$X = C_X^{-2}\left\{2(\beta+64\alpha)-\frac{4}{3}C_X f_X g_X - \frac{2}{3}f_X^2 E^d(X_1)\right\} + E^d(X_1) \quad .$$

Substituting the term C_X as given in (3.22) and rearranging the expression, we finally get

$$\frac{4}{3} f_X (1-\frac{1}{3}f_X^2)^{\frac{1}{2}} g_X = 2(\beta+64\alpha)+E^d(X_1) - X + \left\{\frac{X}{3} - E^d(X_1)\right\} f_X^2 \quad (3.92)$$

with g_X given in (3.59).

Taking the square of both sides of (3.92) and setting

$$\begin{aligned} a_X &= 2(\beta+64\alpha)+E^d(X_1)-X \quad , \\ b_X &= \frac{X}{3} - E^d(X_1) \quad , \end{aligned} \quad (3.93)$$

we obtain

$$\frac{16}{9} g_X^2 f_X^2 - \frac{16}{27} g_X^2 f_X^4 = a_X^2 + 2a_X b_X f_X^2 + b_X^2 f_X^4 ,$$

or

$$\left(b_X^2 + \frac{16}{27} g_X^2\right) f_X^4 + \left(2a_X b_X - \frac{16}{9} g_X^2\right) f_X^2 + a_X^2 = 0 \quad .$$

This is a quadratic equation in f_X^2. Therefore we can obtain the value of f_X^2 to be

$$f_X^2 = \frac{-\left(2a_X b_X - \frac{16}{9} g_X^2\right) \pm \sqrt{\left(2a_X b_X - \frac{16}{9} g_X^2\right)^2 - 4a_X^2\left(b_X^2 + \frac{16}{27} g_X^2\right)}}{2\left(b_X^2 + \frac{16}{27} g_X^2\right)} \tag{3.94}$$

Similarly, substituting $E^S(L_1)$, as given in (3.64), and $E(L_2,)$, as given (3.36), into (3.91), we obtain

$$L = C_L^{-2}\left\{2(\beta + 48\alpha) - \frac{4}{3} C_L f_L g_L - \frac{2}{3} f_L E^d(L_1)\right\} + E^d(L_1) \quad .$$

Substituting C_L as given in (3.23), we finally get

$$\frac{4}{3} f_L \left(1 - \frac{1}{3} f_L^2\right)^{\frac{1}{2}} g_L = 2(\beta + 48\alpha) + E^d(L_1) - L + \left\{\frac{L}{3} - E^d(L_1)\right\} f_L^2 . \tag{3.95}$$

Again, letting

$$\begin{aligned} a_L &= 2(\beta + 48\alpha) + E^d(L_1) - L \quad , \\ b_L &= \frac{L}{3} - E^d(L_1) \quad , \end{aligned} \tag{3.95A}$$

and taking the square of both sides of (3.95), we finally rearrange terms to get

$$\frac{16}{9} g_L^2 f_L^2 - \frac{16}{27} g_L^2 f_L^4 = a_L^2 + 2a_L b_L f_L^2 + b_L^2 f_L^4 ,$$

or

$$\left(b_L^2 + \frac{16}{27} g_L^2\right) f_L^4 + \left(2a_L b_L - \frac{16}{9} g_L^2\right) f_L^2 + a_L^2 = 0 \quad .$$

This is again a quadratic equation in f_L^2, and we obtain

$$f_L^2 = \frac{-(2a_L b_L - \frac{16}{9} g_L^2) \pm \sqrt{(2a_L b_L - \frac{16}{9} g_L^2)^2 - 4a_L^2 (b_L^2 + \frac{16}{27} g_L^2)}}{2(b_L^2 + \frac{16}{27} g_L^2)} \qquad (3.96)$$

The parameter B_4 can now be obtained by taking the ratio of (3.94) and (3.96),

$$\frac{f_X}{f_L} = \frac{j_2(k^X B_4)}{j_2(k^L B_4)} = \left[\frac{(\frac{16}{9} g_X^2 - 2a_X b_X) \pm \sqrt{(\frac{16}{9} g_X^2 - 2a_X b_X)^2 - 4a_X^2 (\frac{16}{27} g_X^2 + b_X^2)}}{(\frac{16}{9} g_L^2 - 2a_L b_L) \pm \sqrt{(\frac{16}{9} g_L^2 - 2a_L b_L)^2 - 4a_L^2 (\frac{16}{27} g_L^2 + b_L^2)}} \times \frac{(\frac{16}{27} g_L^2 + b_L^2)}{(\frac{16}{27} g_X^2 + b_X^2)} \right]^{\frac{1}{2}}, \qquad (3.97)$$

and again iterating on a computer. With B_4 determined, B_5 can be obtained from (3.94) :

$$B_5 = \left[\frac{(\frac{16}{9} g_X^2 - 2a_X b_X) \pm \sqrt{(\frac{16}{9} g_X^2 - 2a_X b_X)^2 - 4a_X^2 (\frac{16}{27} g_X^2 + b_X^2)}}{2(b_X^2 + \frac{16}{27} g_X^2)} \right] \times \left[j_2(k^X B_4) \right]^{-1} . \qquad (3.98)$$

With B_4 and B_5 determined, the parameters V_1 and V_2 appearing in $E(L_{2'})$ and $E(X_{4'})$ can be obtained directly from Eq.(3.36) and Eq.(3.31) :

$$V_1 = \beta + 48\alpha - E(L_{2'})\left(1 - \frac{1}{3}f_L^2\right), \qquad (3.99)$$

and

$$V_2 = \beta + 64\alpha - E(X_{4'})\left(1 - \frac{1}{3}f_X^2\right). \qquad (3.100)$$

It is useful to summarize here the expressions through which the 9 parameters are extracted explicitly:

9. $\beta = E(\Gamma_1)$

10. $\alpha = \frac{\hbar^2}{2m}\left(\frac{\pi}{4a}\right)^2$

11. Solve B_1 from

$$\frac{j_2(k^X B_1)}{j_2(k^W B_1)} = \sqrt{\frac{24}{25}}\sqrt{\frac{\{E^d(X_1)-E(X_{11})\}\{E(X_{12})-E^d(X_1)\}}{\{E^d(W_{2'})-E(W_{21}')\}\{E(W_{22}')-E^d(W_{2'})\}}}$$

12. $B_2 = \sqrt{\frac{3}{2}} \times \sqrt{\{E^d(L_1)-E(L_{11})\}\{E(L_{12})-E^d(L_1)\}} \Big/ j_2(k^L B_1)$

13. $B_3 = \sqrt{\frac{3}{2}} \times \sqrt{\{E^d(X_1)-E(X_{11})\}\{E(X_{12})-E^d(X_1)\}} \Big/ j_2(k^X B_1)$

14. Solve B_4 from

$$\frac{j_2(k^X B_4)}{j_2(k^L B_4)} = \left[\frac{\left(\frac{16}{9}g_X^2-2a_Xb_X\right) \pm \sqrt{\left(\frac{16}{9}g_X^2-2a_Xb_X\right)^2-4a_X^2\left(\frac{16}{27}g_X^2+b_X^2\right)}}{\left(\frac{16}{9}g_L^2-2a_Lb_L\right) \pm \sqrt{\left(\frac{16}{9}g_L^2-2a_Lb_L\right)^2-4a_L^2\left(\frac{16}{27}g_L^2+b_L^2\right)}} \times \frac{\left(\frac{16}{27}g_L^2+b_L^2\right)}{\left(\frac{16}{27}g_X^2+b_X^2\right)}\right]^{\frac{1}{2}}$$

15.
$$\mathcal{B}_5 = \left[\frac{\left(\frac{16}{9}g_X^2 - 2a_X b_X\right) \pm \sqrt{\left(\frac{16}{9}g_X^2 - 2a_X b_X\right)^2 - 4a_X^2\left(\frac{16}{27}g_X^2 + b_X^2\right)}}{2\times\left(\frac{16}{27}g_X^2 + b_X^2\right)}\right] \times \left[j_2(k^X \mathcal{B}_4)\right]^{-1} \qquad (3.101)$$

16. $$V_1 = \beta + 48\alpha - E(L_{2'})\left(1 - \tfrac{1}{3}f_L^2\right)$$

17. $$V_2 = \beta + 64\alpha - E(X_{4'})\left(1 - \tfrac{1}{3}f_X^2\right)$$

It using these expressions, the abbreviations a_X and and b_X are given in (3.93), a_L and b_L in (3.95A), f_X and g_X in (3.22), and f_L and g_L in (3.23).

Eq.(3.9) and Eq.(3.101) constitute our scheme for the explicit extraction of the 17 interpolation parameters.