CHATER IV

THE COMPUTATION, RESULTS, AND DISCUSSIONS

1 The Computation

The Scheme of Computation

The scheme of computation is the demonstration that our interpolation scheme is capable of reproducing the reference band structure for paramagnetic copper. We will demonstrate that the interpolated bands fit the reference bands with good accuracy throughout the Brillouin zone. The reference band structure we chose was that calculated by Burdick for Cu with the APW method[8].

In this scheme of computation, the first step is the extraction of the adjustable parameters. The parameters used in our scheme are computed from eigenvalues at high symmetry points in the Brillouin zone. As there are 17 adjustable parameters in the scheme, 17 energies are therefore needed for the 17 expressions for extracting parameters as listed in Eq.(3.9) and Eq.(3.101) .

The following steps could be followed after the parameters have been obtained:

(i) The Hamiltonian matrix for a given reciprocal lattice vector at a given point in the Brillouin zone is set up in four blocks; namely the diagonal LCAO-LCAO block according to

Eq.(2.29), the diagonal OPW-OPW block according to Eq.(2.50), and the off-diagonal hybridizing OPW-LCAO block according to Eq.(2.56). These blocks form the 9x9 Hamiltonian matrix.

(ii) The 9x9 Hamiltonian matrix is then diagonalized numerically to yield 9 eigenvalues and 9 corresponding eigenvectors for the chosen reciprocal lattice vector.

According to the symmetry at the particular point in the Brillouin zone, some eigenvalues may be degenerate. The point group symmetry of any band will, strictly speaking, have to be determined from the symmetry of the corresponding eigenvector. However, by tracing bands from points of high symmetry for which the symmetries of different bands are known from either experiment or first-principles band calculations, symmetry may be assigned to most bands by inspection. Care, however, has to be exercised in the assignment for those points of the Brillouin zone at which some bands cross or come close to one another.

For detailed comparison of the interpolation scheme band structure with the reference band structure, the nine lowest bands are calculated at 89 points in 1/48 of the primitive cell in the Brillouin zone of the fcc lattice in which $k_y \geq k_x \geq k_z \geq 0$, shown in Fig.2-3 . The band structure is therefore calculated at a very fine mesh, with nearest mesh points seperated by a distance of the order of $\frac{\pi}{4a}$ where a is the lattice constant. The mesh is chosen after Burdick who computed the APW band structure for paramagnetic fcc copper for the same mesh. However, Burdick did not give all nine lowest eigenvalues at each of the mesh points.

This necessitates some extrapolation and interpolation from eigenvalues of nearby mesh points in order to obtain the missing eigenvalues. This process is shown in detail in Appendix D and the extrapolated or interpolated eigenvalues thus obtained are listed in parenthesis in Table 4-1.

To compute the rms deviation of the interpolation band structure from the reference band structure, it was decided that only the 6 lowest eigenvalues at the 89 points in the Brillouin zone in 1/48 of the primitive cell would be used. This is mainly because of the fact that many eigenvalues of the higher (7^{th}, 8^{th}, and 9^{th}) bands were not listed by Burdick, sometime for adjacent points in the Brillouin zone. Extrapolation and interpolation may not give reliable results in this situation.

The Process of Computation

The main computation is performed on an IBM-360 computer of the IBM Company. The programs were written in FORTRAN IV language. The computer programs were not constructed from scratch. The basic programs were adapted from a set made available by the group of Professor Henry Ehrenreich through Dr. Kopr Kritayakirana and it originated from the pioneer work of Laurent Hodges. Owing to differences of the computers employed, some adaptations and amendments in the programs had to be made.

The program consists of two major parts; a main program and subprograms (or subroutines). The main program, which is listed in Appendix C, may be understood from its flow chart, which is also listed in Appendix C. The subroutines, which are called by the main program, perform the major part of mathematical computations of the interpolation scheme. The processes of computation in the computer program can be described briefly as follows:

1. The major input consists of the following:

(i) The 89 reciprocal lattice vectors in 1/48 of the primitive cell in the Brillouin zone at which band energies are to be computed.

(ii) The 17 eigenvalues at points of high symmetry in the Brillouin zone from Burdick's calculation and the lattice constant. These are needed for determining the 17 interpolation parameters.

2. Subroutine PRMFT2 is first called to compute the 17 interpolation parameters. The determination of the parameters in this subroutine follows the sequence of relations indicated in Eqs.(3.9) and (3.101) . We arrange the determination of the parameters into two groups as follows:

The first group of 8 parameters depends only on the 8 eigenvalues of pure d states, as evident from Eq.(3.9) . The values of A_2, A_1, E_o, and A_5 were computed from the simple algebraic expressions involving the eigenvalues at Γ_{12}, $\Gamma_{25'}$, X_5, X_3, and X_2 . The next parameter, A_4, depends on the eigenvalues $E(\Gamma_{12})$ and $E(K_4)$ as well as the value of A_5 just computed previously. Parameter Δ, the cubic crystal field splitting, depends on $E(\Gamma_{12})$, E_o, A_4, and A_5. Parameter A_3 depends on $E(L_{31})$, $E(L_{32})$, E_o, and Δ . To get A_6, we need the values of Δ, $E(L_{31})$, $E(L_{32})$, and A_3 which was just computed.

The second group of the remaining 9 parameters depends on eigenvalues of pure conduction states and hybridized states, as shown in Eq.(3.101). Parameter β, the bottom of the conduction band, was simply taken to be $E(\Gamma_1)$ and parameter α, the width of the conduction band parabola, depends only on the lattice constant in our scheme. Parameter B_1 was obtained through the ratio of two second order spherical Bessel functions, given in Relation 11 in Eq.(3.101). This value of B_1 is computed in Subroutine ARG. The computation is straightforward. Starting with a small trial value of B_1, the ratio of the values of the two second order spherical Bessel functions was taken. If the ratio did not come close to the predetermined ratio, the trial value was increased by a small step and the same process was continued until the ratio was satisfied by the correct trial value which was taken to be the value of B_1. After parameter B_1 was obtained, parameters B_2 and B_3 were then obtained from simple algebraic expressions as given in Relations 12 and 13 in Eq.(3.101). Parameter B_4 was obtained by the same iterative process as that used to obtain B_1. After B_4 was obtained, B_5 was computed from Relation 15. Parameter V_1 and V_2 were computed last after B_4 and B_5 were computed.

3. After the 17 parameters are obtained, the computation enters into the main DO loop. In each loop, a reciprocal lattice vector, $\vec{K}$, is chosen, the 9x9 Hamiltonian matrix is set up for that $\vec{K}$ vector, the matrix is diagonalized to yield 9 eigenvalues and 9 corresponding eigenvectors. The eigenvalues are ordered in increasing energy. The loop is then repeated for a new reciprocal

lattice vector until all 89 reciprocal lattice vectors are exhausted.

3.1 The Hamiltonian matrix is set up in blocks as apparent in Eq.(2.25). The LCAO-LCAO block is set up by Subroutine DDBLOK which is constructed from Eq.(2.29) and listed in Appendix C. The OPW-OPW block and the off-diagonal OPW-LCAO block are set up by Subroutine OPWXD which is constructed from Eqs.(2.50) and (2.56) respectively and listed in Appendix C. Cut-off in the orthogonalization form factor f(k), as shown in Fig.2-4, and cut-off in the hybridization form factor g(k), as shown in Fig.2-5, are effected through Subroutines RF and RG respectively. These subroutines are also listed in Appendix C.

3.2 The Hamiltonian matrix is diagonalized with the help of Subroutine HDIAG. This is a standard FORTRAN IV subroutine for diagonalization of a real symmetric matrix by the Jacobi method. The subroutine can provide both eigenvalues and corresponding eigenvectors.

3.3 The eigenvalues are then arranged in order of increasing values by Subroutine ORDER.

4. The quantities available for output of the program are

(i) the 17 interpolation parameters, and

(ii) the 9 lowest eigenvalues at 89 points in 1/48 of the primitive cell of the Brillouin zone and their corresponding eigenvectors if desired.

5. The overall rms deviation of the 89x6 eigenvalues for the six lowest bands is computed and the maximum deviation in the primitive cell in the Brillouin zone is identified.

2 The Results

The reference band structure which the interpolation scheme tries to reproduce is shown in tabulated form in Table 4-1 and in graphic form in Figs. 4-1 and 4-2. The band structure is given by the nine lowest eigenvalues at 89 points in 1/48 of the primitive cell of the Brillouin zone at mesh point frequency of $\frac{\pi}{4a}$, where $a = 3.6147$ Å (6.83087 a.u.) is the fcc lattice constant of copper. The reference band structure is taken from Burdick's calculation using the APW method as published in Ref. 8. In Burdick's results, 29 eigenvalues in the nine lowest bands are not listed. In order to make use of all 89x6 eigenvalues in computing the rms deviation of the interpolated bands from Burdick's APW bands, the missing values from Burdick's listing were obtained by extrapolation and interpolation of eigenvalues of nearby points in the Brillouin zone. The details of the extrapolation and interpolation processes are shown in Appendix D. For each eigenvalue determined this way, extrapolation and/or interpolation were done from as many directions as possible and consistency of different extrapolations/interpolations for the same eigenvalue was carefully attempted as a check of the precision of the extrapolation/interpolation. The greatest deviation between different extrapolations/interpolations is the eigenvalue for the 6^{th} band associated with the point (343) in the Brillouin zone. Extrapolating along a line consisting of eigenvalues associated with the points (340), (341) and (342) by spacing of equal steps and of steps proportional to length of the $\vec{k}$-vectors, value of -0.5020 and -0.5330 Rydbergs were obtained respectively for the point (343). We settled on the value of -0.5020 Rydberg for the point (343) for the 6^{th} band.

The values of the 17 interpolation parameters in our scheme obtained from fitting the reference bands as discussed in Section 4-1 are listed in Table 4-2. For comparison purposes, the values of the 15 interpolation parameters in Hodges' interpolation scheme are also listed.

Band energies of paramagnetic fcc copper which are computed by our hybrid interpolation scheme for the nine lowest eigenvalues at 89 points in 1/48 of the primitive cell in the Brillouin zone are listed in Table 4-3. The eigenvalues, expressed in rydbergs, are computed with the computer program listed in Appendix C and the reciprocal lattice vectors $\vec{K}$ are expressed in units of $\frac{\pi}{4a}$. We also computed an interpolated band structure without including the orthogonalization effects. This is just Hodges' scheme. The band energies of paramagnetic fcc copper computed by interpolation scheme in the case of neglecting orthogonalization effects (Hodges' scheme) are listed in Table 4-4. All eigenvalues of the nine lowest bands at 89 points in 1/48 of the primitive cell of the Brillouin zone are expressed in rydbergs and the reciprocal lattice vectors $\vec{K}$ in units of $\frac{\pi}{4a}$. This computation was carried out using the computer program listed in Appendix C for only 15 parameters; namely, E_o, Δ, $A_1, \ldots, A_6$, α, β, V_1, V_2, B_1, B_2, B_3. B_4 and B_5 were set equal to zero.

The deviations between our interpolation eigenvalues and reference eigenvalues are listed in Table 4-5.

The greatest deviation occurs at (381) and its value is marked with a parenthesis. The overall rms deviation of these two bands is also computed to be 0.18 eV.

To compare the working of the different schemes of interpolation, we interpolated band energies of the lowest nine levels at Γ, X, L, W, and some other points on symmetry lines in the Brillouin zone. The results for these different schemes of computation; namely Mueller's, Hodges', and the hybrid scheme of the present work, are compared with the calculated values of Burdick (Ref. 8) in Table 4-6.

Table 4-1

Reference band structure

Paramagnetic copper band energies from Burdick's APW calculation (Ref. 8) for the lowest 9 bands at 89 points in 1/48 of the primitive cell in the Brillouin zone. All band energies are given in rydbergs. The values listed in parenthesis are obtained by extrapolation or interpolation as described in Appendix D. The first column specifies the $\vec{k}$ vectors expressed in units of $\frac{\pi}{4a}$; the second column specifies $w(\vec{k})$ which is the number of "like" vectors in the Brillouin zone; the other columns give the band energies.

	$\vec{k}$	w	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9
Γ	000	1	-1.0430	-0.6400	-0.6400	-0.6400	-0.5820	-0.5820	1.3320	1.4210	1.4210
	010	6	-1.0290	-0.6450	-0.6380	-0.6380	-0.5860	-0.5810	1.2940	1.3610	1.3610
	020	6	-0.9890	-0.6570	-0.6300	-0.6300	-0.5980	-0.5780	1.1950	1.1950	1.2130
	030	6	-0.9290	-0.6740	-0.6160	-0.6160	-0.6100	-0.5740	1.0350	1.0350	1.1360
	040	6	-0.8590	-0.6960	-0.6110	-0.5970	-0.5970	-0.5680	0.8910	0.8910	0.9920
	050	6	-0.7910	-0.7150	-0.5740	-0.5740	-0.5670	-0.5600	0.7330	0.7690	0.7690
	060	6	-0.7730	-0.7290	-0.5510	-0.5510	-0.5490	-0.4560	0.4780	0.6750	0.6750
	070	6	-0.7750	-0.7380	-0.5450	-0.5340	-0.5340	-0.3180		0.6150	0.6150
X	080	3	-0.7760	-0.7390	-0.5400	-0.5270	-0.5270	-0.2350	0.1520	0.6010	0.6010
	110	12	-1.0190	-0.6480	-0.6360	-0.6360	-0.5870	-0.5830	1.1780	1.2230	1.4290
	120	24	-0.9590	-0.6590	-0.6390	-0.6290	-0.5990	-0.5890	1.0310	1.0660	1.4390
	130	24	-0.8890	-0.6750	-0.6290	-0.6160	-0.6090	-0.5790	0.9060	0.9240	1.2860
	140	24	-0.8290	-0.6940	-0.6290	-0.5970	-0.5890	-0.5690	0.7840	0.7970	1.0200
	150	24	-0.7820	-0.7120	-0.6120	-0.5740	-0.5690	-0.5290	0.6770	0.6910	0.7510
	160	24	-0.7660	-0.7260	-0.5810	-0.5590	-0.5510	-0.4240	0.4890	0.5940	0.6110
	170	24	-0.7680	-0.7350	-0.5590	-0.5490	-0.5340	-0.2880	0.2700	0.5410	0.5580
	180	12	-0.7710	-0.7360	-0.5460	-0.5460	-0.5270	-0.2030	0.1570	0.5210	0.5390
	220	12	-0.9390	-0.6640	-0.6310	-0.6240	-0.6000	-0.5750	0.8840	0.9110	1.5100
	230	24	-0.8690	-0.6750	-0.6390	-0.6140	-0.6090	-0.5590	0.7510	0.7740	1.4890
	240	24	-0.8060	-0.6890	-0.6450	-0.5960	-0.5910	-0.5290	0.6300	0.6540	1.0410
	250	24	-0.7560	-0.7030	-0.6440	-0.5750	-0.5740	-0.4690	0.5280	0.6110	0.7790
	260	24	-0.7460	-0.7150	-0.6220	-0.5610	-0.5510	-0.3600	0.4490	0.4810	0.5210
	270	24	-0.7510	-0.7220	-0.5990	-0.5590	-0.5340	-0.2180	0.2940	0.4010	0.4410
	280	12	-0.7540	-0.7230	-0.5880	-0.5590	-0.5270	-0.1240	0.1740	0.3610	0.4320
	330	12	-0.8290	-0.6770	-0.6410	-0.6090	-0.6060	-0.5280	0.6120	0.6400	1.3820
	340	24	-0.7650	-0.6820	-0.6560	-0.6040	-0.5930	-0.4790	0.4880	0.5300	
	350	24	-0.7240	-0.6890	-0.6690	-0.5880	-0.5730	-0.4020	0.3880	0.4460	0.8310
	360	24	-0.7200	-0.6960	-0.6590	-0.5780	-0.5510	-0.2810	0.3090	0.3910	0.5740
	370	24	-0.7290	-0.7020	-0.6410	-0.5770	-0.5350	-0.1390	0.2570	0.3310	0.3510
	380	12	-0.7340	-0.7020	-0.6320	-0.5760	-0.5270	-0.0180	0.2060	0.2410	0.3310
	440	12	-0.7270	-0.6750	-0.6670	-0.6070	-0.5840	-0.4160	0.3660	0.4310	1.1430
	450	24	-0.7190	-0.6790	-0.6720	-0.5990	-0.5690	-0.3200	0.2610		
	460	24	-0.7090	-0.6890	-0.6710	-0.5890	-0.5510	-0.1880	0.1770	0.3020	0.6490

	$\vec{k}$	w	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9
	470	24	-0.7190	-0.6790	-0.6720	-0.5870	-0.5350	-0.0280	0.1250	0.2700	0.4150
W	480	6	-0.7230	-0.6710	-0.6710	-0.5850	-0.5270	0.1050	0.1050	0.2450	0.2730
	550	12	-0.7090	-0.6890	-0.6530	-0.5940	-0.5620	-0.2120	0.1410	0.9230	
	560	24	-0.7190	-0.6990	-0.6410	-0.5850	-0.5480	-0.0760	0.0810	0.2420	0.7270
	570	8	-0.7290	-0.7090	-0.6350	-0.5790	-0.5350	0.0020	0.0870	0.2010	0.5050
K	660	4	-0.7340	-0.7110	-0.6120	-0.5720	-0.5430	-0.0330	0.0590	0.1860	0.7490
	111	8	-1.0040	-0.6500	-0.6340	-0.6340	-0.5860	-0.5860	1.0290	1.3610	1.3930
	121	24	-0.9390	-0.6690	-0.6390	-0.6300	-0.5990	-0.5890	0.8750		
	131	24	-0.8790	-0.6730	-0.6290	-0.6210	-0.5990	-0.5790	0.7350	1.0810	
	141	24	-0.8290	-0.6910	-0.6340	-0.6060	-0.5690	-0.5660	0.6150	0.9190	1.0110
	151	24	-0.7740	-0.7070	-0.6210	-0.5910	-0.5490	-0.5090	0.5180	0.7550	0.8000
	161	24	-0.7600	-0.7290	-0.5910	-0.5720	-0.5390	-0.4010	0.4410	0.5010	0.7110
	171	24	-0.7690	-0.7390	-0.5670	-0.5590	-0.5390	-0.2630	0.2780	0.3930	0.6520
	181	12	-0.7690	-0.7330	-0.5580	-0.5500	-0.5310	-0.1740	0.1640	0.3760	0.6350
	221	24	-0.9090	-0.6690	-0.6390	-0.6290	-0.5990	-0.5790	0.7170	1.0810	
	231	48	-0.8490	-0.6790	-0.6390	-0.6290	-0.5890	-0.5600	0.5760	0.9610	
	241	48	-0.8000	-0.6810	-0.6420	-0.6100	-0.5690	-0.5280	0.4810	0.8410	1.0810
	251	48	-0.7540	-0.6960	-0.6430	-0.5970	-0.5510	-0.4690	0.3630	0.7210	0.8010
	261	48	-0.7490	-0.7090	-0.6240	-0.5790	-0.5390	-0.3490	0.2870	0.5310	0.6670
	271	48	-0.7440	-0.7170	-0.6020	-0.5670	-0.5380	-0.1990	0.2510	0.3310	0.6180
	281	24	-0.7480	-0.7210	-0.5940	-0.5640	-0.5340	(-0.0990)	0.1610	0.2410	0.6020
	331	24	-0.8190	-0.6690	-0.6490	-0.6230	-0.5890	-0.5390	0.4400	0.8320	
	341	48	-0.7680	-0.6660	-0.6520	-0.6170	-0.5770	-0.4690	0.3230	0.7180	
	351	48	-0.7330	-0.6790	-0.6590	-0.6030	-0.5580	-0.3970	0.2290	0.6410	0.8410
	361	48	-0.7200	-0.6950	-0.6520	-0.5880	-0.5460	-0.2710	0.1570	0.5610	0.6010
	371	48	-0.7240	-0.7000	-0.6400	-0.5800	-0.5380	-0.1160	0.1110	0.3510	0.5180
	381	16	-0.7290	-0.7090	-0.6350	-0.5790	-0.5350	0.0870	0.2110	0.5050	
	441	24	-0.7410	-0.6690	-0.6590	-0.6170	-0.5730	-0.4160	0.2080	0.6090	
	451	48	-0.7200	-0.6780	-0.6510	-0.6080	-0.5590	-0.3160	0.1210	0.5250	0.9130
	461	48	-0.7030	-0.6970	-0.6560	-0.5960	-0.5480	-0.1840	0.0450	0.4810	0.6590
	471	24	-0.7130	-0.6870	-0.6630	-0.5870	-0.5380	-0.0420	0.0190	0.4220	0.4310
	551	24	-0.7190	-0.6890	-0.6490	-0.6040	-0.5540	-0.2120	0.0240	0.4430	0.9310
	561	24	-0.7170	-0.6960	-0.6400	-0.5920	-0.5460	-0.1070	-0.0160		

	$\vec{k}$	w	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9
	222	8	-0.8890	-0.6580	-0.6300	-0.6300	-0.5800	-0.5800	0.5570	1.3020	1.3090
	232	24	-0.8290	-0.6590	-0.6390	-0.6300	-0.5790	-0.5650	0.4150		
	242	24	-0.7890	-0.6690	-0.6490	-0.6240	-0.5500	-0.5290	0.3010	1.0080	1.0810
	252	24	-0.7510	-0.6810	-0.6430	-0.6130	-0.5400	-0.4320	0.2050	0.8150	0.8950
	262	24	-0.7390	-0.6980	-0.6390	-0.5970	-0.5360	-0.3090	0.1210	0.5620	0.8130
	272	24	-0.7390	-0.7090	-0.6180	-0.5820	-0.5390	-0.1490	0.0840	0.3360	0.7630
U	282	8	-0.7390	-0.7110	-0.6120	-0.5720	-0.5430	-0.0350	0.0590	0.2060	0.7490
	332	24	-0.8070	-0.6390	-0.6390	-0.6340	(-0.5720)	-0.5410	0.2810	1.0410	
	342	48	-0.7740	-0.6480	-0.6330	-0.6250	-0.5560	-0.4790	0.1660	0.9370	
	352	48	-0.7460	-0.6670	-0.6330	-0.6190	-0.5430	-0.3890	0.0810	0.8410	0.8810
	362	48	-0.7270	-0.6860	-0.6370	-0.6070	-0.5390	-0.2480	0.0070	0.6160	0.7860
	372	24	-0.7170	-0.6970	-0.6400	-0.5920	-0.5460	-0.1070	-0.0160	0.3880	0.7440
	442	24	-0.7590	-0.6540	-0.6320	-0.6090	-0.5550	-0.4170	0.0540	0.8380	
	452	48	-0.7420	-0.6670	-0.6240	-0.6180	-0.5470	-0.3160	-0.0250	0.7610	0.9470
	462	48	-0.7230	-0.6830	-0.6360	-0.6100	-0.5440	-0.2110		0.6870	0.7070
	552	12	-0.7350	-0.6740	-0.6240	-0.6190	-0.5430	-0.2530	-0.0640	0.6760	0.9740
	333	8	-0.7920	-0.6380	-0.6380	-0.5730	-0.5530	-0.5530	0.1460	1.2240	1.2590
	343	24	-0.7740	-0.7060	-0.6450	-0.5890	-0.5790	(-0.5020)		1.1510	1.1510
	353	24	-0.7560	-0.6580	-0.6310	-0.6020	-0.5380	(-0.4030)	-0.0410	0.9240	1.0410
	363	12	-0.7350	-0.6740	-0.6240	-0.6190	-0.5430	-0.2530	-0.0650		0.9740
	443	24	-0.7710	-0.6460	-0.6390	-0.5620	-0.5430	-0.4230	-0.0530	1.0810	
	453	24	-0.7600	-0.6550	-0.6340	-0.5860	-0.5390	-0.3520	-0.0850	0.9770	1.0190
L	444	4	-0.7750	-0.6420	-0.6420	-0.5380	-0.5380	-0.4290	-0.0940	1.1910	1.5020

Table 4-2. Values of interpolation scheme parameters used for fitting Burdick's APW bands for paramagnetic copper with the hybrid interpolation scheme. For comparison purposes, parameters for Hodges' scheme are also shown.

Parameter	Hybrid	Hodges
E_o	-0.60825	-0.60825
Δ	-0.00445	-0.00445
A_1	0.02031	0.02031
A_2	0.00619	0.00619
A_3	0.01024	0.01024
A_4	0.01292	0.01292
A_5	0.00262	0.00262
A_6	0.00827	0.00827
α	0.01322	0.01540
β	-1.04300	-1.04300
$V_1 = V_{111}$	-0.00778	0.12507
$V_2 = V_{200}$	0.02393	0.17743
$B_1 = R_1$	0.41981	0.36899
$B_2 = K_2$	0.93760	1.03638
$B_3 = K_3$	0.97929	1.03638
$B_4 = R_o$	0.47370	—
$B_5 = K_o$	1.45227	—

Table 4-3

Cu band structure computed in the interpolation scheme of the present work. The format of the Table is the same as that of Table 4-1.

	$\vec{k}$	w	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9
Γ	000	1	-1.0430	-0.6400	-0.6400	-0.6400	-0.5820	-0.5820	1.4952	1.4952	2.3413
	010	6	-1.0298	-0.6438	-0.6357	-0.6357	-0.5866	-0.5804	1.2969	1.2969	1.9315
	020	6	-0.9902	-0.6545	-0.6235	-0.6235	-0.5985	-0.5759	1.1251	1.1251	1.5481
	030	6	-0.9258	-0.6706	-0.6109	-0.6051	-0.6051	-0.5690	0.9796	0.9796	1.1912
	040	6	-0.8461	-0.6895	-0.6069	-0.5835	-0.5835	-0.5610	0.8608	0.8611	0.8611
	050	6	-0.7858	-0.7084	-0.5619	-0.5619	-0.5530	-0.5484	0.5776	0.7699	0.7716
	060	6	-0.7672	-0.7245	-0.5462	-0.5435	-0.5435	-0.4302	0.3692	0.7063	0.7099
	070	6	-0.7698	-0.7352	-0.5416	-0.5313	-0.5313	-0.3000	0.2139	0.6691	0.6741
X	080	3	-0.7761	-0.7390	-0.5400	-0.5270	-0.5270	-0.2350	0.1502	0.6569	0.6623
	110	12	-1.0166	-0.6453	-0.6333	-0.6322	-0.5880	-0.5814	1.0981	1.0991	1.9447
	120	24	-0.9771	-0.6541	-0.6231	-0.6222	-0.5974	-0.5766	0.9262	0.9274	1.5613
	130	24	-0.9129	-0.6685	-0.6191	-0.6043	-0.5984	-0.5675	0.7834	0.7834	1.2044
	140	24	-0.8338	-0.6858	-0.6179	-0.5829	-0.5795	-0.5547	0.6684	0.6729	0.8741
	150	24	-0.7753	-0.7030	-0.5901	-0.5615	-0.5569	-0.5162	0.5742	0.5920	0.5957
	160	24	-0.7583	-0.7177	-0.5651	-0.5460	-0.5434	-0.4053	0.3699	0.5267	0.5373
	170	24	-0.7615	-0.7276	-0.5510	-0.5417	-0.5313	-0.2725	0.2062	0.4952	0.5055
	180	12	-0.7688	-0.7311	-0.5447	-0.5426	-0.5270	-0.2026	0.1361	0.4871	0.4942
	220	12	-0.9380	-0.6563	-0.6215	-0.6154	-0.6017	-0.5707	0.7567	0.7592	1.6010
	230	24	-0.8748	-0.6642	-0.6250	-0.6028	-0.6005	-0.5556	0.6200	0.6242	1.2440
	240	24	-0.7987	-0.6757	-0.6319	-0.5886	-0.5809	-0.5306	0.5101	0.5244	0.9136
	250	24	-0.7460	-0.6882	-0.6201	-0.5693	-0.5605	-0.4713	0.4275	0.4522	0.6242
	260	24	-0.7343	-0.6996	-0.5985	-0.5581	-0.5430	-0.3515	0.3421	0.4030	0.4314
	270	24	-0.7399	-0.7083	-0.5836	-0.5563	-0.5312	-0.2078	0.1895	0.3718	0.3814
	280	12	-0.7491	-0.7142	-0.5788	-0.5579	-0.5270	-0.1192	0.0991	0.3604	0.3799
	330	12	-0.8153	-0.6618	-0.6278	-0.6132	-0.5913	-0.5326	0.4887	0.5012	1.3101
	340	24	-0.7486	-0.6639	-0.6403	-0.6046	-0.5762	-0.4933	0.3862	0.4109	0.9796
	350	24	-0.7076	-0.6694	-0.6462	-0.5863	-0.5585	-0.4122	0.3105	0.3372	0.6837
	360	24	-0.7038	-0.6766	-0.6351	-0.5751	-0.5423	-0.2810	0.2537	0.2801	0.4543
	370	24	-0.7142	-0.6854	-0.6240	-0.5743	-0.5311	-0.1294	0.1696	0.2457	0.3340
	380	12	-0.7276	-0.6958	-0.6221	-0.5772	-0.5270	-0.0070	0.0612	0.2375	0.3235
	440	12	-0.7045	-0.6563	-0.6472	-0.6127	-0.5673	-0.4313	0.2931	0.3143	1.0722
	450	24	-0.6832	-0.6636	-0.6522	-0.6003	-0.5546	-0.3290	0.2275	0.2317	0.7709
	460	24	-0.6843	-0.6712	-0.6540	-0.5888	-0.541[illegible]	-0.[illegible]944	0.1682	0.1926	0.5224

	k		Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9
	470	24	-0.7041	-0.6639	-0.6603	-0.5865	-0.5309	-0.0533	0.1290	0.1666	0.3581
W	480	6	-0.7192	-0.6656	-0.6656	-0.5885	-0.5270	0.0469	0.1170	0.1170	0.3085
	550	12	-0.6945	-0.6715	-0.6402	-0.5971	-0.5481	-0.2185	0.1409	0.1836	0.8872
	560	24	-0.7089	-0.6877	-0.6311	-0.5854	-0.5391	-0.0935	0.0652	0.1741	0.6238
	570	8	-0.7223	-0.6961	-0.6253	-0.5783	-0.5306	0.0128	0.0167	0.1969	0.4271
K	660	4	-0.7336	-0.7077	-0.6055	-0.5720	-0.5355	-0.0273	0.0074	0.1935	0.7582
	111	8	-1.0034	-0.6464	-0.6304	-0.6304	-0.5854	-0.5854	0.9003	1.3234	1.9579
	121	24	-0.9642	-0.6533	-0.6232	-0.6221	-0.5939	-0.5783	0.7327	1.1515	1.5745
	131	24	-0.9006	-0.6656	-0.6226	-0.6093	-0.5889	-0.5678	0.5983	1.0061	1.2176
	141	24	-0.8231	-0.6808	-0.6235	-0.5938	-0.5616	-0.5559	0.4948	0.8872	0.8872
	151	24	-0.7671	-0.6964	-0.5992	-0.5777	-0.5446	-0.5021	0.4182	0.6008	0.7963
	161	24	-0.7521	-0.7103	-0.5721	-0.5633	-0.5358	-0.3860	0.3409	0.4110	0.7331
	171	24	-0.7557	-0.7205	-0.5578	-0.5530	-0.5306	-0.2489	0.1960	0.3582	0.6960
	181	12	-0.7628	-0.7260	-0.5541	-0.5492	-0.5289	-0.1728	0.1195	0.3519	0.6839
	221	24	-0.9259	-0.6536	-0.6220	-0.6204	-0.5925	-0.5733	0.5749	0.9796	1.6142
	231	48	-0.8649	-0.6585	-0.6270	-0.6141	-0.5848	-0.5578	0.4514	0.8349	1.2573
	241	48	-0.7934	-0.6675	-0.6333	-0.6021	-0.5635	-0.5318	0.3566	0.7202	0.9268
	251	48	-0.7459	-0.6797	-0.6209	-0.5863	-0.5460	-0.4627	0.2788	0.6305	0.6395
	261	48	-0.7343	-0.6927	-0.6008	-0.5718	-0.5366	-0.3357	0.2183	0.4138	0.5768
	271	48	-0.7379	-0.7051	-0.5882	-0.5637	-0.5318	-0.1885	0.1479	0.2792	0.5435
	281	24	-0.7457	-0.7153	-0.5855	-0.5616	-0.5301	-0.0945	0.0760	0.2557	0.5331
	331	24	-0.8108	-0.6516	-0.6288	-0.6212	-0.5810	-0.5349	0.3363	0.6953	1.3234
	341	48	-0.7546	-0.6489	-0.6393	-0.6125	-0.5664	-0.4931	0.2380	0.5868	0.9929
	351	48	-0.7208	-0.6629	-0.6360	-0.5962	-0.5500	-0.4038	0.1616	0.5066	0.6959
	361	48	-0.7102	-0.6774	-0.6284	-0.5837	-0.5392	-0.2660	0.1069	0.4354	0.4751
	371	48	-0.7127	-0.6904	-0.6235	-0.5787	-0.5329	-0.1127	0.0695	0.2758	0.4328
	381	16	-0.7223	-0.6962	-0.6253	-0.5783	-0.5306	0.0128	0.0177	0.1960	0.4271
	441	24	-0.7245	-0.6471	-0.6307	-0.6189	-0.5611	-0.4273	0.1438	0.4847	1.0854
	451	48	-0.7075	-0.6628	-0.6297	-0.6065	-0.5498	-0.3188	0.0690	0.4112	0.7836
	461	48	-0.6952	-0.6814	-0.6356	-0.5943	-0.5398	-0.1779	0.0166	0.3608	0.5333
	471	24	-0.6985	-0.6810	-0.6467	-0.5881	-0.5333	-0.0562	0.0127	0.2925	0.3859
	551	24	-0.7098	-0.6720	-0.6261	-0.6029	-0.5446	-0.2048	-0.0044	0.3442	0.9003
	561	24	-0.7126	-0.6875	-0.6251	-0.5900	-0.5378	-0.0800	-0.0554	0.3020	0.6356

	k	w	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9
	222	8	-0.8907	-0.6479	-0.6241	-0.6241	-0.5769	-0.5769	0.4310	1.2308	1.6539
	232	24	-0.8371	-0.6431	-0.6307	-0.6222	-0.5678	-0.5610	0.3153	1.0854	1.2969
	242	24	-0.7795	-0.6497	-0.6306	-0.6147	-0.5476	-0.5268	0.2176	0.9664	0.9664
	252	24	-0.7430	-0.6655	-0.6191	-0.6030	-0.5383	-0.4338	0.1405	0.6714	0.8741
	262	24	-0.7302	-0.6817	-0.6080	-0.5893	-0.5342	-0.2927	0.0832	0.4395	0.8091
	272	24	-0.7291	-0.6986	-0.6039	-0.5773	-0.5344	-0.1375	0.0436	0.2714	0.7709
U	282	8	-0.7336	-0.7077	-0.6055	-0.5720	-0.5355	-0.0273	0.0074	0.1935	0.7582
	332	24	-0.7985	-0.6313	-0.6311	-0.6207	-0.5647	-0.5418	0.2005	0.9400	1.3630
	342	48	-0.7630	-0.6442	-0.6258	-0.6064	-0.5506	-0.4917	0.1056	0.8220	1.0325
	352	48	-0.7393	-0.6598	-0.6172	-0.6057	-0.5400	-0.3820	0.0293	0.7311	0.7347
	362	48	-0.7241	-0.6748	-0.6160	-0.6001	-0.5367	-0.2294	-0.0300	0.4875	0.6713
	372	24	-0.7127	-0.6875	-0.6250	-0.5900	-0.5378	-0.0801	-0.0548	0.3016	0.6355
	442	24	-0.7502	-0.6462	-0.6301	-0.5918	-0.5499	-0.4207	0.0167	0.7078	1.1251
	452	48	-0.7385	-0.6592	-0.6208	-0.5994	-0.5421	-0.3055	-0.0567	0.6226	0.8220
	462	24	-0.7220	-0.6728	-0.6159	-0.6069	-0.5386	-0.1709	-0.1037	0.5551	0.5738
	552	12	-0.7355	-0.6656	-0.6149	-0.6047	-0.5389	-0.2216	-0.1058	0.5421	0.9400
	333	8	-0.7829	-0.6358	-0.6358	-0.5697	-0.5504	-0.5504	0.0927	1.2176	1.4291
	343	24	-0.7677	-0.6439	-0.6341	-0.5692	-0.5407	-0.4781	0.0050	1.0986	1.0986
	353	24	-0.7538	-0.6552	-0.6265	-0.5855	-0.5369	-0.3562	-0.0646	0.7963	1.0061
	363	12	-0.7355	-0.6657	-0.6149	-0.6046	-0.5389	-0.2215	-0.1061	0.5421	0.9400
	443	24	-0.7681	-0.6436	-0.6388	-0.5560	-0.5412	-0.4230	-0.0658	0.9797	1.1912
	453	24	-0.7599	-0.6516	-0.6320	-0.5744	-0.5384	-0.3424	-0.1015	0.8868	0.8876
T.	444	4	-0.7750	-0.6420	-0.6420	-0.5380	-0.5380	-0.4290	-0.0940	1.2837	1.2837

Table 4-4

Paramagnetic copper energy eigenvalues in rydbergs at 89 points for nine lowest bands computed with our interpolation scheme without including orthogonalization effects (Hodges' scheme). Its format is the same as that of Table 4-1.

	K	W	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9
Γ	000	1	-1.0430	-0.6400	-0.6400	-0.6400	-0.5820	-0.5820	1.9133	1.9133	2.8987
	010	6	-1.0277	-0.6438	-0.6357	-0.6357	-0.5866	-0.5804	1.6823	1.6823	2.4214
	020	6	-0.9826	-0.6545	-0.6235	-0.6235	-0.5990	-0.5759	1.4822	1.4822	1.9749
	030	6	-0.9115	-0.6706	-0.6134	-0.6051	-0.6051	-0.5690	1.3128	1.3128	1.5594
	040	6	-0.8272	-0.6895	-0.6148	-0.5835	-0.5835	-0.5610	1.1742	1.1742	1.1757
	050	6	-0.7687	-0.7084	-0.5647	-0.5619	-0.5619	-0.5530	0.8277	1.0664	1.0664
	060	6	-0.7588	-0.7245	-0.5462	-0.5435	-0.5435	-0.4456	0.5247	0.9894	0.9894
	070	6	-0.7680	-0.7352	-0.5416	-0.5313	-0.5313	-0.3086	0.2911	0.9433	0.9433
X	080	3	-0.7760	-0.7390	-0.5400	-0.5270	-0.5270	-0.2350	0.1900	0.9279	0.9279
	110	12	-1.0125	-0.6453	-0.6333	-0.6323	-0.5880	-0.5814	1.4478	1.4550	2.4368
	120	24	-0.9679	-0.6541	-0.6232	-0.6222	-0.5979	-0.5767	1.2469	1.2555	1.9903
	130	24	-0.8975	-0.6686	-0.6197	-0.6043	-0.6002	-0.5678	1.0765	1.0871	1.5747
	140	24	-0.8145	-0.6858	-0.6217	-0.5829	-0.5819	-0.5558	0.9365	0.9492	1.1912
	150	24	-0.7587	-0.7031	-0.5935	-0.5616	-0.5582	-0.5249	0.8190	0.8268	0.8657
	160	24	-0.7502	-0.7178	-0.5657	-0.5463	-0.5434	-0.4175	0.5292	0.7467	0.7757
	170	24	-0.7597	-0.7278	-0.5516	-0.5422	-0.5313	-0.2821	0.2942	0.6956	0.7353
	180	12	-0.7689	-0.7316	-0.5447	-0.5440	-0.5270	-0.2116	0.1956	0.6716	0.7312
	220	12	-0.9248	-0.6565	-0.6218	-0.6154	-0.6017	-0.5718	1.0342	1.0682	2.0365
	230	24	-0.8573	-0.6645	-0.6251	-0.6037	-0.6006	-0.5580	0.8612	0.9027	1.6208
	240	24	-0.7795	-0.6762	-0.6329	-0.5898	-0.5809	-0.5354	0.7177	0.7688	1.2370
	250	24	-0.7321	-0.6889	-0.6213	-0.5697	-0.5605	-0.4796	0.6031	0.6632	0.8909
	260	24	-0.7289	-0.7005	-0.5996	-0.5585	-0.5430	-0.3612	0.5162	0.5236	0.6552
	270	24	-0.7407	-0.7099	-0.5866	-0.5568	-0.5312	-0.2205	0.3008	0.4554	0.6123
	280	12	-0.7542	-0.7177	-0.5842	-0.5579	-0.5270	-0.1482	0.1970	0.4178	0.6371
	330	12	-0.7968	-0.6632	-0.6283	-0.6132	-0.5913	-0.5376	0.6699	0.7586	1.6977
	340	24	-0.7323	-0.6655	-0.6408	-0.6048	-0.5762	-0.5002	0.5225	0.6317	1.3132
	350	24	-0.6993	-0.6714	-0.6461	-0.5866	-0.5586	-0.4201	0.4032	0.5376	0.9638
	360	24	-0.7046	-0.6800	-0.6352	-0.5760	-0.5424	-0.2880	0.3111	0.4566	0.6782
	370	24	-0.7222	-0.6915	-0.6287	-0.5748	-0.5311	-0.1381	0.2458	0.2994	0.5795
	380	12	-0.7427	-0.7070	-0.6325	-0.5762	-0.5270	-0.0565	0.1907	0.2093	0.6198
	440	12	-0.6945	-0.6600	-0.6487	-0.6127	-0.5673	-0.4399	0.3572	0.5357	1.4206
	450	24	-0.6795	-0.6663	-0.6575	-0.6007	-0.5547	-0.3383	0.2362	0.4563	1.0681
	460	24	-0.6941	-0.6688	-0.6617	-0.5895	-0.5413	-0.1989	0.1438	0.4055	0.7643

	$\vec{k}$	w	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9
	470	24	-0.7200	-0.6717	-0.6688	-0.5859	-0.5310	-0.0430	0.0821	0.3065	0.6087
W	480	6	-0.7399	-0.6798	-0.6798	-0.5859	-0.5270	0.0581	0.0581	0.1916	0.6208
	550	12	-0.6898	-0.6832	-0.6494	-0.5971	-0.5481	-0.2291	0.1070	0.4125	1.2050
	560	24	-0.7135	-0.6954	-0.6421	-0.5853	-0.5392	-0.0921	0.0168	0.3853	0.8876
	570	8	-0.7373	-0.7021	-0.6365	-0.5780	-0.5307	-0.0390	0.0577	0.3327	0.6723
K	660	4	-0.7404	-0.7156	-0.6153	-0.5720	-0.5355	-0.0730	0.0291	0.3795	1.0510
	111	8	-0.9976	-0.6467	-0.6304	-0.6304	-0.5854	-0.5854	1.2205	1.7131	2.4522
	121	24	-0.9536	-0.6538	-0.6233	-0.6221	-0.5944	-0.5783	1.0204	1.5130	2.0057
	131	24	-0.8845	-0.6661	-0.6230	-0.6093	-0.5911	-0.5678	0.8511	1.3436	1.5902
	141	24	-0.8039	-0.6811	-0.6261	-0.5938	-0.5662	-0.5559	0.7122	1.2050	1.2065
	151	24	-0.7518	-0.6966	-0.6025	-0.5777	-0.5446	-0.5120	0.6017	0.8598	1.0972
	161	24	-0.7450	-0.7108	-0.5734	-0.5633	-0.5358	-0.3989	0.4898	0.5895	1.0202
	171	24	-0.7546	-0.7218	-0.5598	-0.5530	-0.5306	-0.2619	0.2886	0.5111	0.9741
	181	12	-0.7647	-0.7282	-0.5569	-0.5492	-0.5289	-0.1887	0.1856	0.5045	0.9587
	221	24	-0.9119	-0.6553	-0.6222	-0.6204	-0.5925	-0.5739	0.8209	1.3131	2.0519
	231	48	-0.8472	-0.6603	-0.6271	-0.6142	-0.5858	-0.5596	0.6523	1.1439	1.6362
	241	48	-0.7753	-0.6682	-0.6342	-0.6023	-0.5646	-0.5367	0.5146	1.0053	1.2523
	251	48	-0.7333	-0.6806	-0.6218	-0.5864	-0.5462	-0.4723	0.4071	0.8844	0.9165
	261	48	-0.7291	-0.6958	-0.6020	-0.5721	-0.5367	-0.3487	0.3231	0.6005	0.8257
	271	48	-0.7385	-0.7100	-0.5921	-0.5640	-0.5318	-0.2060	0.2248	0.4189	0.7828
	281	24	-0.7527	-0.7204	-0.5921	-0.5616	-0.5302	-0.1283	0.1395	0.3947	0.7751
	331	24	-0.7929	-0.6544	-0.6290	-0.6212	-0.5810	-0.5393	0.4854	0.9775	1.7131
	341	48	-0.7403	-0.6505	-0.6398	-0.6126	-0.5666	-0.5004	0.3505	0.8406	1.3286
	351	48	-0.7127	-0.6657	-0.6365	-0.5964	-0.5502	-0.4151	0.2479	0.7337	0.9792
	361	48	-0.7075	-0.6842	-0.6300	-0.5844	-0.5393	-0.2820	0.1756	0.6162	0.7166
	371	48	-0.7197	-0.6969	-0.6294	-0.5791	-0.5329	-0.1341	0.1162	0.4116	0.6637
	381	16	-0.7365	-0.7029	-0.6365	-0.5780	-0.5307	-0.0396	0.0516	0.3332	0.6784
	441	24	-0.7161	-0.6483	-0.6348	-0.6189	-0.5611	-0.4385	0.2197	0.7141	1.4360
	451	48	-0.7028	-0.6660	-0.6351	-0.6070	-0.5499	-0.3368	0.1237	0.6153	1.0834
	461	48	-0.6934	-0.6894	-0.6422	-0.5948	-0.5398	-0.2053	0.0641	0.5404	0.7807
	471	24	-0.7128	-0.6845	-0.6555	-0.5882	-0.5333	-0.0884	0.0514	0.4076	0.6414
	551	24	-0.7056	-0.6806	-0.6348	-0.6029	-0.5446	-0.2369	0.0341	0.5396	1.2204
	561	24	-0.7092	-0.7004	-0.6341	-0.5902	-0.537[illegible]	-0.1515	0.0159	0.4871	0.9030

	$\vec{k}$	w	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6	Band 7	Band 8	Band 9
	222	8	-0.8747	-0.6528	-0.6241	-0.6241	-0.5769	-0.5769	0.6241	1.6053	2.0981
	232	24	-0.8195	-0.6475	-0.6308	-0.6222	-0.5696	-0.5610	0.4579	1.4360	1.6824
	242	24	-0.7646	-0.6506	-0.6319	-0.6147	-0.5476	-0.5332	0.3243	1.2974	1.2984
	252	24	-0.7339	-0.6680	-0.6198	-0.6030	-0.5383	-0.4468	0.2237	0.9490	1.1896
	262	24	-0.7249	-0.6892	-0.6106	-0.5893	-0.5342	-0.3155	0.1533	0.6474	1.1126
	272	24	-0.7283	-0.7096	-0.6102	-0.5773	-0.5344	-0.1702	0.0933	0.4385	1.0664
U	282	8	-0.7404	-0.7156	-0.6153	-0.5720	-0.5355	-0.0730	0.0291	0.3795	1.0510
	332	24	-0.7835	-0.6314	-0.6311	-0.6260	-0.5647	-0.5443	0.2994	1.2672	1.7593
	342	48	-0.7532	-0.6444	-0.6259	-0.6082	-0.5507	-0.4994	0.1735	1.1288	1.3748
	352	48	-0.7330	-0.6616	-0.6179	-0.6076	-0.5400	-0.4008	0.0852	1.0099	1.0346
	362	48	-0.7188	-0.6828	-0.6203	-0.6006	-0.5367	-0.2706	0.0356	0.7112	0.9479
	372	24	-0.7095	-0.7014	-0.6331	-0.5902	-0.5378	-0.1479	0.0165	0.4818	0.9044
	442	24	-0.7447	-0.6464	-0.6301	-0.5951	-0.5499	-0.4352	0.0619	0.9041	1.4822
	452	48	-0.7340	-0.6605	-0.6210	-0.6049	-0.5421	-0.3388	-0.0075	0.8879	1.1295
	462	24	-0.7176	-0.6782	-0.6232	-0.6072	-0.5386	-0.2466	-0.0126	0.7755	0.8517
	552	12	-0.7313	-0.6698	-0.6149	-0.6118	-0.5389	-0.2837	-0.0372	0.7927	1.2666
	333	8	-0.7735	-0.6358	-0.6358	-0.5756	-0.5504	-0.5504	0.1508	1.5899	1.8363
	343	24	-0.7634	-0.6438	-0.6341	-0.5696	-0.5407	-0.4846	0.0378	1.4514	1.4517
	353	24	-0.7502	-0.6557	-0.6265	-0.5883	-0.5369	-0.3799	-0.0289	1.0998	1.3436
	363	12	-0.7312	-0.6707	-0.6149	-0.6110	-0.5390	-0.2816	-0.0354	0.7888	1.2666
	443	24	-0.7665	-0.6434	-0.6388	-0.5564	-0.5412	-0.4314	-0.0503	1.3136	1.5591
	453	24	-0.7573	-0.6516	-0.6320	-0.5770	-0.5384	-0.3673	-0.0729	1.1989	1.2129
L	444	4	-0.7750	-0.6420	-0.6420	-0.5380	-0.5380	-0.4290	-0.0940	1.6669	1.6669

Table 4-5

Deviation of the interpolated bands from the reference bands. At each $\vec{k}$ point, the first row specifies eigenvalues of the reference bands, the second row specifies eigenvalues of the interpolated bands, and the third row gives values of deviation of these two eigenvalues at that point. All values are listed in rydbergs. Deviation values marked with one asterisk are those between 0.01 to 0.02 rydbergs. Values marked with two asterisks are those between 0.02 to 0.03 rydbergs. Values marked with three asterisks are those greater than 0.03 rydberg. Maximum deviation value is listed in a parenthesis.

$\vec{k}$	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6
000	-1.0430	-0.6400	-0.6400	-0.6400	-0.5820	-0.5820
	-1.0430	-0.6400	-0.6400	-0.6400	-0.5820	-0.5820
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
010	-1.0290	-0.6450	-0.6380	-0.6380	-0.5860	-0.5810
	-1.0298	-0.6438	-0.6357	-0.6357	-0.5866	-0.5804
	0.0008	-0.0012	-0.0023	-0.0023	0.0006	-0.0006
020	-0.9890	-0.6570	-0.6300	-0.6300	-0.5980	-0.5780
	-0.9902	-0.6545	-0.6235	-0.6235	-0.5985	-0.5759
	0.0012	-0.0025	-0.0065	-0.0065	0.0005	-0.0021
030	-0.9290	-0.6740	-0.6160	-0.6160	-0.6100	-0.5740
	-0.9258	-0.6706	-0.6109	-0.6051	-0.6051	-0.5690
	-0.0032	-0.0034	-0.0051	-0.0109*	-0.0049	-0.0050
040	-0.8590	-0.6960	-0.6110	-0.5970	-0.5970	-0.5680
	-0.8461	-0.6895	-0.6069	-0.5835	-0.5835	-0.5610
	-0.0129*	-0.0065	-0.0041	-0.0135*	-0.0135*	-0.0070
050	-0.7910	-0.7150	-0.5740	-0.5740	-0.5670	-0.5600
	-0.7858	-0.7084	-0.5619	-0.5619	-0.5530	-0.5484
	-0.0052	-0.0066	-0.0121*	-0.0121*	-0.0140*	-0.0116*
060	-0.7730	-0.7290	-0.5510	-0.5510	-0.5490	-0.4560
	-0.7672	-0.7245	-0.5462	-0.5435	-0.5435	-0.4302
	-0.0058	-0.0045	-0.0048	-0.0075	-0.0055	-0.0258*
070	-0.7750	-0.7380	-0.5450	-0.5340	-0.5340	-0.3180
	-0.7698	-0.7352	-0.5416	-0.5313	-0.5313	-0.3000
	-0.0052	-0.0028	-0.0034	-0.0037	-0.0027	-0.0180*
080	-0.7760	-0.7390	-0.5400	-0.5270	-0.5270	-0.2350
	-0.7761	-0.7390	-0.5400	-0.5270	-0.5270	-0.2350
	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
110	-1.0190	-0.6480	-0.6360	-0.6360	-0.5870	-0.5830
	-1.0166	-0.6453	-0.6333	-0.6322	-0.5880	-0.5814
	-0.0024	-0.0027	-0.0027	-0.0038	0.0010	-0.0016

$\vec{k}$	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6
120	-0.9590	-0.6590	-0.6390	-0.6290	-0.5990	-0.5890
	-0.9771	-0.6541	-0.6231	-0.6222	-0.5974	-0.5766
	0.0181*	-0.0049	-0.0159*	-0.0068	-0.0016	-0.0124*
130	-0.8890	-0.6750	-0.6290	-0.6160	-0.6090	-0.5790
	-0.9129	-0.6685	-0.6191	-0.6043	-0.5984	-0.5675
	0.0239**	-0.0065	-0.0099	-0.0117*	-0.0106*	-0.0115*
140	-0.8290	-0.6940	-0.6290	-0.5970	-0.5890	-0.5690
	-0.8338	-0.6858	-0.6179	-0.5829	-0.5795	-0.5547
	0.0048	-0.0082	-0.0111*	-0.0141*	-0.0095	-0.0143*
150	-0.7820	-0.7120	-0.6120	-0.5740	-0.5690	-0.5290
	-0.7753	-0.7030	-0.5901	-0.5615	-0.5569	-0.5162
	-0.0067	-0.0090	-0.0219**	-0.0125*	-0.0121*	-0.0128*
160	-0.7660	-0.7260	-0.5810	-0.5590	-0.5510	-0.4240
	-0.7583	-0.7177	-0.5651	-0.5460	-0.5434	-0.4053
	-0.0077	-0.0083	-0.0159*	-0.0130*	-0.0076	-0.0187*
170	-0.7680	-0.7350	-0.5590	-0.5490	-0.5340	-0.2880
	-0.7615	-0.7276	-0.5510	-0.5417	-0.5313	-0.2725
	-0.0065	-0.0074	-0.0080	-0.0073	-0.0027	-0.0155*
180	-0.7710	-0.7360	-0.5460	-0.5460	-0.5270	-0.2030
	-0.7688	-0.7311	-0.5447	-0.5426	-0.5270	-0.2026
	-0.0022	-0.0049	-0.0013	-0.0034	0.0000	-0.0004
220	-0.9390	-0.6640	-0.6310	-0.6240	-0.6000	-0.5750
	-0.9380	-0.6563	-0.6215	-0.6154	-0.6017	-0.5707
	-0.0010	-0.0077	-0.0095	-0.0086	0.0017	-0.0043
230	-0.8690	-0.6750	-0.6390	-0.6140	-0.6090	-0.5590
	-0.8748	-0.6642	-0.6250	-0.6028	-0.6005	-0.5556
	0.0058	-0.0108*	-0.0140*	-0.0112*	-0.0085	-0.0034
240	-0.8060	-0.6890	-0.6450	-0.5960	-0.5910	-0.5290
	-0.7987	-0.6757	-0.6319	-0.5886	-0.5809	-0.5306
	-0.0073	-0.0133*	-0.0131*	-0.0074	-0.0101*	0.0016

$\vec{k}$	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6
250	-0.7560	-0.7030	-0.6440	-0.5750	-0.5740	-0.4690
	-0.7460	-0.6882	-0.6201	-0.5693	-0.5605	-0.4713
	-0.0100	-0.0148*	-0.0239**	-0.0057	-0.0135*	0.0023
260	-0.7460	-0.7150	-0.6220	-0.5610	-0.5510	-0.3600
	-0.7343	-0.6996	-0.5985	-0.5581	-0.5430	-0.3515
	-0.0117*	-0.0154*	-0.0235**	-0.0029	-0.0080	-0.0085
270	-0.7510	-0.7220	-0.5990	-0.5590	-0.5340	-0.2180
	-0.7399	-0.7083	-0.5836	-0.5563	-0.5312	-0.2078
	-0.0111*	-0.0137*	-0.0154*	-0.0027	-0.0028	-0.0102*
280	-0.7540	-0.7230	-0.5880	-0.5590	-0.5270	-0.1240
	-0.7491	-0.7142	-0.5788	-0.5579	-0.5270	-0.1192
	-0.0049	-0.0088	-0.0092	-0.0011	0.0000	-0.0048
330	-0.8290	-0.6770	-0.6410	-0.6090	-0.6060	-0.5280
	-0.8153	-0.6618	-0.6278	-0.6132	-0.5913	-0.5326
	-0.0137*	-0.0152*	-0.0132*	0.0042	-0.0157*	0.0046
340	-0.7650	-0.6820	-0.6560	-0.6040	-0.5930	-0.4790
	-0.7486	-0.6639	-0.6403	-0.6046	-0.5762	-0.4933
	-0.0164*	-0.0181*	-0.0157*	0.0006	-0.0168*	0.0143*
350	-0.7240	-0.6890	-0.6690	-0.5880	-0.5730	-0.4020
	-0.7076	-0.6694	-0.6462	-0.5863	-0.5585	-0.4122
	-0.0164*	-0.0196*	-0.0228**	-0.0017	-0.0145*	0.0102*
360	-0.7200	-0.6960	-0.6590	-0.5780	-0.5510	-0.2810
	-0.7038	-0.6766	-0.6351	-0.5751	-0.5423	-0.2810
	-0.0162*	-0.0194*	-0.0239**	-0.0029	-0.0087	0.0000
370	-0.7290	-0.7020	-0.6410	-0.5770	-0.5350	-0.1390
	-0.7142	-0.6854	-0.6240	-0.5743	-0.5311	-0.1294
	-0.0148*	-0.0166*	-0.0170*	-0.0027	-0.0039	-0.0096
380	-0.7340	-0.7020	-0.6320	-0.5760	-0.5270	-0.0180
	-0.7276	-0.6958	-0.6221	-0.5772	-0.5270	-0.0070
	-0.0064	-0.0062	-0.0099	0.0012	0.0000	-0.0110*

$\vec{k}$	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6
440	-0.7270	-0.6750	-0.6670	-0.6070	-0.5840	-0.4160
	-0.7045	-0.6563	-0.6472	-0.6127	-0.5673	-0.4313
	-0.0225 **	-0.0187 *	-0.0198 *	0.0057	-0.0167*	0.0153 *
450	-0.7190	-0.6790	-0.6720	-0.5990	-0.5690	-0.3200
	-0.6832	-0.6636	-0.6522	-0.6003	-0.5546	-0.3290
	-0.0358 ***	-0.0154 *	-0.0198 *	0.0013	-0.0144*	0.0090
460	-0.7090	-0.6890	-0.6710	-0.5890	-0.5510	-0.1880
	-0.6843	-0.6712	-0.6540	-0.5888	-0.5412	-0.1944
	-0.0247 **	-0.0178 *	-0.0170 *	-0.0002	-0.0098	0.0064
470	-0.7190	-0.6790	-0.6720	-0.5870	-0.5350	-0.0280
	-0.7041	-0.6639	-0.6603	-0.5865	-0.5309	-0.0533
	-0.0149 *	-0.0151 *	-0.0117 *	-0.0005	-0.0041	0.0253 **
480	-0.7230	-0.6710	-0.6710	-0.5850	-0.5270	0.1050
	-0.7192	-0.6656	-0.6656	-0.5885	-0.5270	0.0469
	-0.0038	-0.0054	-0.0054	0.0035	0.0000	0.0581***
550	-0.7090	-0.6890	-0.6530	-0.5940	-0.5620	-0.2120
	-0.6945	-0.6715	-0.6402	-0.5971	-0.5481	-0.2185
	-0.0145 *	-0.0175 *	-0.0128 *	0.0031	-0.0139*	0.0065
560	-0.7190	-0.6990	-0.6410	-0.5850	-0.5480	-0.0760
	-0.7089	-0.6877	-0.6311	-0.5854	-0.5391	-0.0935
	-0.0101 *	-0.0113 *	-0.0099	0.0004	-0.0089	0.0175 *
570	-0.7290	-0.7090	-0.6350	-0.5790	-0.5350	0.0020
	-0.7223	-0.6961	-0.6253	-0.5783	-0.5306	0.0128
	-0.0067	-0.0129 *	-0.0097	-0.0007	-0.0044	-0.0108 *
660	-0.7340	-0.7110	-0.6120	-0.5720	-0.5430	-0.0330
	-0.7336	-0.7077	-0.6055	-0.5720	-0.5355	-0.0273
	-0.0004	-0.0033	-0.0065	0.0000	-0.0075	-0.0057
111	-1.0040	-0.6500	-0.6340	-0.6340	-0.5860	-0.5860
	-1.0034	-0.6464	-0.6304	-0.6304	-0.5854	-0.5854
	-0.0006	-0.0036	-0.0036	-0.0036	-0.0006	-0.0006

$\vec{k}$	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6
121	-0.9390	-0.6690	-0.6390	-0.6300	-0.5990	-0.5890
	-0.9642	-0.6533	-0.6232	-0.6221	-0.5939	-0.5783
	0.0252**	-0.0157*	-0.0158*	-0.0079	-0.0051	-0.0107*
131	-0.8790	-0.6730	-0.6290	-0.6210	-0.5990	-0.5790
	-0.9006	-0.6656	-0.6226	-0.6093	-0.5889	-0.5678
	0.0216**	-0.0074	-0.0064	-0.0117*	-0.0101*	-0.0112*
141	-0.8290	-0.6910	-0.6340	-0.6060	-0.5690	-0.5660
	-0.8231	-0.6808	-0.6235	-0.5938	-0.5616	-0.5559
	-0.0059	-0.0102*	-0.0105*	-0.0122*	-0.0074	-0.0101*
151	-0.7740	-0.7070	-0.6210	-0.5910	-0.5490	-0.5090
	-0.7671	-0.6964	-0.5992	-0.5777	-0.5446	-0.5021
	-0.0069	-0.0106*	-0.0218**	-0.0133*	-0.0044	-0.0069
161	-0.7600	-0.7290	-0.5910	-0.5720	-0.5390	-0.4010
	-0.7521	-0.7103	-0.5721	-0.5633	-0.5358	-0.3860
	-0.0079	-0.0187*	-0.0189*	-0.0087	-0.0032	-0.0150*
171	-0.7690	-0.7390	-0.5670	-0.5590	-0.5390	-0.2630
	-0.7557	-0.7205	-0.5578	-0.5530	-0.5306	-0.2489
	-0.0133*	-0.0185*	-0.0092	-0.0060	-0.0084	-0.0141*
181	-0.7690	-0.7330	-0.5580	-0.5500	-0.5310	-0.1740
	-0.7628	-0.7260	-0.5541	-0.5492	-0.5289	-0.1728
	-0.0062	-0.0070	-0.0039	-0.0008	-0.0021	-0.0012
221	-0.9090	-0.6690	-0.6390	-0.6290	-0.5990	-0.5790
	-0.9259	-0.6536	-0.6220	-0.6204	-0.5925	-0.5733
	0.0169*	-0.0154*	-0.0170*	-0.0086	-0.0065	-0.0057
231	-0.8490	-0.6790	-0.6390	-0.6290	-0.5890	-0.5600
	-0.8649	-0.6585	-0.6270	-0.6141	-0.5848	-0.5578
	0.0159*	-0.0205**	-0.0120*	-0.0149*	-0.0042	-0.0022
241	-0.8000	-0.6810	-0.6420	-0.6100	-0.5690	-0.5280
	-0.7934	-0.6675	-0.6333	-0.6021	-0.5635	-0.5318
	-0.0066	-0.0135*	-0.0087	-0.0079	-0.0055	0.0038

$\vec{k}$	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6
251	-0.7540	-0.6960	-0.6430	-0.5970	-0.5510	-0.4690
	-0.7459	-0.6797	-0.6209	-0.5863	-0.5460	-0.4627
	-0.0081	-0.0163 *	-0.0221 **	-0.0107 *	-0.0050	-0.0063
261	-0.7490	-0.7090	-0.6240	-0.5790	-0.5390	-0.3490
	-0.7343	-0.6927	-0.6008	-0.5718	-0.5366	-0.3357
	-0.0147 *	-0.0163 *	-0.0232 **	-0.0072	-0.0024	-0.0133 *
271	-0.7440	-0.7170	-0.6020	-0.5670	-0.5380	-0.1990
	-0.7379	-0.7051	-0.5882	-0.5637	-0.5318	-0.1885
	-0.0061	-0.0119 *	-0.0138 *	-0.0033	-0.0062	-0.0105 *
281	-0.7480	-0.7210	-0.5940	-0.5640	-0.5340	-0.0990
	-0.7457	-0.7153	-0.5855	-0.5616	-0.5301	-0.0945
	-0.0023	-0.0057	-0.0085	-0.0024	-0.0039	-0.0045
331	-0.8190	-0.6690	-0.6490	-0.6230	-0.5890	-0.5390
	-0.8108	-0.6516	-0.6288	-0.6212	-0.5810	-0.5349
	-0.0082	-0.0174 *	-0.0202 **	-0.0018	-0.0080	-0.0041
341	-0.7680	-0.6660	-0.6520	-0.6170	-0.5770	-0.4690
	-0.7546	-0.6489	-0.6393	-0.6125	-0.5664	-0.4931
	-0.0134 *	-0.0171 *	-0.0127 *	-0.0045	-0.0106	0.0241 **
351	-0.7330	-0.6790	-0.6590	-0.6030	-0.5580	-0.3970
	-0.7208	-0.6629	-0.6360	-0.5962	-0.5500	-0.4038
	-0.0122 *	-0.0161 *	-0.0230 **	-0.0068	-0.0080	0.0068
361	-0.7200	-0.6950	-0.6520	-0.5880	-0.5460	-0.2710
	-0.7102	-0.6774	-0.6284	-0.5837	-0.5392	-0.2660
	-0.0098	-0.0176 *	-0.0236 **	-0.0043	-0.0068	-0.0050
371	-0.7240	-0.7000	-0.6400	-0.5800	-0.5380	-0.1160
	-0.7127	-0.6904	-0.6235	-0.5787	-0.5329	-0.1127
	-0.0113 *	-0.0096	-0.0165 *	-0.0013	-0.0051	-0.0033
381	-0.7290	-0.7090	-0.6350	-0.5790	-0.5350	0.0870
	-0.7223	-0.6962	-0.6253	-0.5783	-0.5306	0.0128
	-0.0067	-0.0128 *	-0.0097	-0.0007	-0.0044	(0.0742) ***

$\vec{k}$	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6
441	-0.7410	-0.6690	-0.6590	-0.6170	-0.5730	-0.4160
	-0.7245	-0.6471	-0.6307	-0.6189	-0.5611	-0.4273
	-0.0165*	-0.0219**	-0.0283**	-0.0019	-0.0119*	0.0113*
451	-0.7200	-0.6780	-0.6510	-0.6080	-0.5590	-0.3160
	-0.7075	-0.6628	-0.6297	-0.6065	-0.5498	-0.3188
	-0.0125*	-0.0152*	-0.0213**	-0.0015	-0.0092	0.0028
461	-0.7030	-0.6970	-0.6560	-0.5960	-0.5480	-0.1840
	-0.6952	-0.6814	-0.6356	-0.5943	-0.5398	-0.1779
	-0.0078	-0.0156*	-0.0204**	-0.0017	-0.0082	-0.0061
471	-0.7130	-0.6870	-0.6630	-0.5870	-0.5380	-0.0420
	-0.6985	-0.6810	-0.6467	-0.5881	-0.5333	-0.0562
	-0.0145*	-0.0060	-0.0163*	0.0011	-0.0047	0.0142*
551	-0.7190	-0.6890	-0.6490	-0.6040	-0.5540	-0.2120
	-0.7098	-0.6720	-0.6261	-0.6029	-0.5446	-0.2048
	-0.0092	-0.0170*	-0.0229**	-0.0011	-0.0094	-0.0072
561	-0.7170	-0.6960	-0.6400	-0.5920	-0.5460	-0.1070
	-0.7126	-0.6875	-0.6251	-0.5900	-0.5378	-0.0800
	-0.0044	-0.0085	-0.0149*	-0.0020	-0.0082	-0.0270**
222	-0.8890	-0.6580	-0.6300	-0.6300	-0.5800	-0.5800
	-0.8907	-0.6479	-0.6241	-0.6241	-0.5769	-0.5769
	0.0017	-0.0101*	-0.0059	-0.0059	-0.0031	-0.0031
232	-0.8290	-0.6590	-0.6390	-0.6300	-0.5790	-0.5650
	-0.8371	-0.6431	-0.6307	-0.6222	-0.5678	-0.5610
	0.0081	-0.0159*	-0.0083	-0.0078	-0.0112*	-0.0040
242	-0.7890	-0.6690	-0.6490	-0.6240	-0.5500	-0.5290
	-0.7795	-0.6497	-0.6306	-0.6147	-0.5476	-0.5268
	-0.0095	-0.0193*	-0.0184*	-0.0093	-0.0024	-0.0022
252	-0.7510	-0.6810	-0.6430	-0.6130	-0.5400	-0.4320
	-0.7430	-0.6655	-0.6191	-0.6030	-0.5383	-0.4338
	-0.0080	-0.0155*	-0.0239**	-0.0100	-0.0017	0.0018

$\vec{k}$	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6
262	-0.7390	-0.6980	-0.6390	-0.5970	-0.5360	-0.3090
	-0.7302	-0.6817	-0.6080	-0.5893	-0.5342	-0.2927
	-0.0088	-0.0063	-0.0310 ***	-0.0077	-0.0018	-0.0163 *
272	-0.7390	-0.7090	-0.6180	-0.5820	-0.5390	-0.1490
	-0.7291	-0.6986	-0.6039	-0.5773	-0.5344	-0.1375
	-0.0099	-0.0104 *	-0.0141 *	-0.0047	-0.0046	-0.0115 *
282	-0.7390	-0.7110	-0.6120	-0.5720	-0.5430	-0.0350
	-0.7336	-0.7077	-0.6055	-0.5720	-0.5355	-0.0273
	-0.0054	-0.0033	-0.0065	0.0000	-0.0075	-0.0077
332	-0.8070	-0.6390	-0.6390	-0.6340	-0.5720	-0.5410
	-0.7985	-0.6313	-0.6311	-0.6207	-0.5647	-0.5418
	-0.0085	-0.0077	-0.0079	-0.0133 *	-0.0073	0.0008
342	-0.7740	-0.6480	-0.6330	-0.6250	-0.5560	-0.4790
	-0.7630	-0.6442	-0.6258	-0.6064	-0.5506	-0.4917
	-0.0110 *	-0.0038	-0.0072	-0.0186 *	-0.0054	0.0127
352	-0.7460	-0.6670	-0.6330	-0.6190	-0.5430	-0.3890
	-0.7393	-0.6598	-0.6172	-0.6057	-0.5400	-0.3820
	-0.0067	-0.0072	-0.0158 *	-0.0133 *	-0.0030	-0.0070
362	-0.7270	-0.6860	-0.6370	-0.6070	-0.5390	-0.2480
	-0.7241	-0.6748	-0.6160	-0.6001	-0.5367	-0.2294
	-0.0029	-0.0112 *	-0.0210 **	-0.0069	-0.0023	-0.0186 *
372	-0.7170	-0.6970	-0.6400	-0.5920	-0.5460	-0.1070
	-0.7127	-0.6875	-0.6250	-0.5900	-0.5378	-0.0801
	-0.0043	-0.0095	-0.0150 *	-0.0020	-0.0082	-0.0269 **
442	-0.7590	-0.6540	-0.6320	-0.6090	-0.5550	-0.4170
	-0.7502	-0.6462	-0.6301	-0.5918	-0.5499	-0.4207
	-0.0088	-0.0078	-0.0019	-0.0172 *	-0.0051	0.0037
452	-0.7420	-0.6670	-0.6240	-0.6180	-0.5470	-0.3160
	-0.7385	-0.6592	-0.6208	-0.5994	-0.5421	-0.3055
	-0.0035	-0.0078	-0.0032	-0.0186 *	-0.0049	-0.0105 *

$\vec{k}$	Band 1	Band 2	Band 3	Band 4	Band 5	Band 6
462	-0.7230	-0.6830	-0.6360	-0.6100	-0.5440	-0.2110
	-0.7220	-0.6728	-0.6159	-0.6069	-0.5386	-0.1709
	-0.0010	-0.0102 *	-0.0201 **	-0.0031	-0.0054	-0.0401 ***
552	-0.7350	-0.6740	-0.6240	-0.6190	-0.5430	-0.2530
	-0.7355	-0.6656	-0.6149	-0.6047	-0.5389	-0.2216
	0.0005	-0.0084	-0.0091	-0.0143 *	-0.0041	-0.0314 ***
333	-0.7920	-0.6380	-0.6380	-0.5730	-0.5530	-0.5530
	-0.7829	-0.6358	-0.6358	-0.5697	-0.5504	-0.5504
	-0.0091	-0.0022	-0.0022	-0.0033	-0.0026	-0.0026
343	-0.7740	-0.7060	-0.6450	-0.5890	-0.5790	-0.5020
	-0.7677	-0.6439	-0.6341	-0.5692	-0.5407	-0.4781
	-0.0063	-0.0621 ***	-0.0109 *	-0.0198 *	-0.0383 ***	-0.0239 **
353	-0.7560	-0.6580	-0.6310	-0.6020	-0.5380	-0.4030
	-0.7538	-0.6552	-0.6265	-0.5855	-0.5369	-0.3562
	-0.0022	-0.0028	-0.0045	-0.0165 *	-0.0011	-0.0468 ***
363	-0.7350	-0.6740	-0.6240	-0.6190	-0.5430	-0.2530
	-0.7355	-0.6657	-0.6149	-0.6046	-0.5389	-0.2215
	0.0005	-0.0083	-0.0091	-0.0144 *	-0.0041	-0.0315 ***
443	-0.7710	-0.6460	-0.6390	-0.5620	-0.5430	-0.4230
	-0.7681	-0.6436	-0.6388	-0.5560	-0.5412	-0.4230
	-0.0029	-0.0024	-0.0002	-0.0060	-0.0018	0.0000
453	-0.7600	-0.6550	-0.6340	-0.5860	-0.5390	-0.3520
	-0.7599	-0.6516	-0.6320	-0.5744	-0.5384	-0.3424
	-0.0001	-0.0034	-0.0020	-0.0116 *	-0.0006	-0.0096
444	-0.7750	-0.6420	-0.6420	-0.5380	-0.5380	-0.4290
	-0.7750	-0.6420	-0.6420	-0.5380	-0.5380	-0.4290
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table 4-6 Comparison of band energies at certain points in the Brillouin zone for eigenvalues calculated with the different schemes of interpolation and those of Burdick calculated with the APW method. Levels marked with an asterisk were used for fitting in the Hodges and the hybrid schemes. Rms deviations from the Burdick bands are computed for those bands values which are not used for fitting.

POINT		LEVEL	BURDICK	MUELLER	HODGES	HYBRID
000	*	Γ_1	-1.0430	-1.0430	-1.0430	-1.0430
	*	$\Gamma_{25'}$	-0.6400	-0.6470	-0.6400	-0.6400
	*	Γ_{12}	-0.5820	-0.5740	-0.5820	-0.5820
080	*	X_{11}	-0.7760	-0.7760	-0.7760	-0.7761
	*	X_3	-0.7390	-0.7400	-0.7390	-0.7390
	*	X_2	-0.5400	-0.5350	-0.5400	-0.5400
	*	X_5	-0.5270	-0.5340	-0.5270	-0.5270
	*	$X_{4'}$	-0.2350	-0.2430	-0.2350	-0.2350
	*	X_{12}	0.1520	0.1450	0.1900	0.1502
444	*	L_{11}	-0.7750	-0.7740	-0.7750	-0.7750
	*	L_{31}	-0.6420	-0.6480	-0.6420	-0.6420
	*	L_{32}	-0.5380	-0.5430	-0.5380	-0.5380
	*	$L_{2'}$	-0.4290	-0.4350	-0.4290	-0.4290
	*	L_{12}	-0.0940	-0.0990	-0.0940	-0.0940
480	*	$W_{2'1}$	-0.7230	-0.7180	-0.7399	-0.7192
		W_3	-0.6710	-0.6760	-0.6798	-0.6656

POINT	LEVEL	BURDICK	MUELLER	HODGES	HYBRID
	W_1	-0.5850	-0.5830	-0.5859	-0.5885
	$W_{1'}$	-0.5270	-0.5360	-0.5270	-0.5270
	W_3	0.1050	0.1160	0.0581	0.1170
	* $W_{2'2}$	0.2450		0.1916	0.1170
660	K_1	-0.7340		-0.7404	-0.7336
	K_1	-0.7110		-0.7156	-0.7077
	K_3	-0.6120		-0.6153	-0.6055
	* K_4	-0.5720	-0.5720	-0.5720	-0.5720
	K_2	-0.5430		-0.5355	-0.5355
	K_3	-0.0330		-0.0730	-0.0273
282	U_1	-0.7390		-0.7404	-0.7336
	U_1	-0.7110		-0.7156	-0.7077
	U_3	-0.6120		-0.6153	-0.6055
	U_4	-0.5720		-0.5720	-0.5720
	U_2	-0.5430		-0.5355	-0.5355
	U_3	-0.0350		-0.0730	-0.0273
020	Δ_1	-0.9890		-0.9826	-0.9902
	$\Delta_{2'}$	-0.6570		-0.6545	-0.6545
	Δ_5	-0.6300		-0.6235	-0.6235
	Δ_1	-0.5980		-0.5990	-0.5985
	Δ_2	-0.5780		-0.5759	-0.5759
040	Δ_1	-0.8590		-0.8272	-0.8461
	$\Delta_{2'}$	-0.6960		-0.6895	-0.6895
	Δ_1	-0.6110		-0.6148	-0.6069

POINT	LEVEL	BURDICK	MUELLER	HODGES	HYBRID
	Δ_5	-0.5970		-0.5835	-0.5835
	Δ_2	-0.5680		-0.5610	-0.5610
060	Δ_1	-0.7730		-0.7588	-0.7672
	$\Delta_{2'}$	-0.7290		-0.7245	-0.7245
	Δ_5	-0.5510		-0.5462	-0.5462
	Δ_2	-0.5490		-0.5435	-0.5435
	Δ_1	-0.4560		-0.4456	-0.4302
222	Λ_1	-0.8890		-0.8747	-0.8907
	Λ_1	-0.6580		-0.6528	-0.6479
	Λ_3	-0.6300		-0.6241	-0.6241
	Λ_3	-0.5800		-0.5769	-0.5769
280	Z_1	-0.7540		-0.7542	-0.7491
	Z_4	-0.7230		-0.7177	-0.7142
	Z_3	-0.5880		-0.5842	-0.5788
	Z_1	-0.5590		-0.5579	-0.5579
	Z_2	-0.5270		-0.5270	-0.5270
	Z_3	-0.1240		-0.1482	-0.1192
220	Σ_1	-0.9390		-0.9248	-0.9380
	Σ_3	-0.6640		-0.6565	-0.6563
	Σ_1	-0.6310		-0.6218	-0.6215
	Σ_2	-0.6240		-0.6154	-0.6154
	Σ_4	-0.6000		-0.6017	-0.6017
	Σ_1	-0.5750		-0.5718	-0.5707
440	Σ_1	-0.7270		-0.6945	-0.7045

OINT	LEVEL	BURDICK	MUELLER	HODGES	HYBRID
	Σ_3	-0.6750		-0.6600	-0.6563
	Σ_1	-0.6670		-0.6487	-0.6472
	Σ_4	-0.6070		-0.6127	-0.6127
	Σ_2	-0.5840		-0.5673	-0.5673
	Σ_1	-0.4160		-0.4399	-0.4313
462	Q_+	-0.7230		-0.7176	-0.7220
	Q_-	-0.6830		-0.6782	-0.6782
	Q_+	-0.6360		-0.6232	-0.6159
	Q_-	-0.6100		-0.6072	-0.6069
	Q_+	-0.5440		-0.5386	-0.5386
	Q_-	-0.2110		-0.2466	-0.1709
rms deviation from Burdick bands				0.015	0.008 (ry.)
				0.200	0.106 (eV)

Figure 4-1

Comparison of the interpolated bands with the reference bands of Cu. The curves denote the APW bands of Burdick (reference bands) and the dots give the band energies obtained in the present interpolation scheme (interpolated bands).

Figure 4-2

Comparison of Burdick's bands for Cu (reference bands) with the interpolated bands obtained in Hodges' scheme. The curves denote the reference bands while the dotes give the band energies in Hodges' scheme as computed in the present work.

3 Discussions

The main results of our computation appear in Table 4-3 and Fig. 4-1 in which is shown the band structure for paramagnetic fcc copper calculated with our interpolation scheme with parameters obtained through fitting band energies at high symmetry points in the Brillouin zone with first-principles calculated values of Burdick. The reference band structure is also shown in Fig. 4-1. The degree of success of our interpolation scheme in reproducing the reference band structure may be seen from Table 4-5 and Table 4-6 which list the deviation of the interpolated bands from the reference bands. This deviation is also displayed in Fig. 4-1

As can be seen from Table 4-5 and Fig. 4-1, the interpolated band structure reproduces the reference band structure with remarkable accuracy throughout the Brillouin zone even though the band structure is very complicated. Along major symmetry lines in the Brillouin zone; namely, Δ, Λ, Σ, Z, and S, the interpolated bands reproduce the reference bands with good accuracy. For instance, as indicated in Table 4-5, the largest deviation along Δ is approximately 0.026 rydberg for the 6^{th} band at $\vec{k}$ = (060). The largest deviation along Λ is approximately 0.010 rydberg for the 2^{nd} band at $\vec{k}$ = (222), etc. The closeness of the interpolated bands to the reference bands is less impressive along general directions or lines of lower symmetry in the Brillouin zone.

From Table 4-5, it can be seen that of the 89x6=534 pairs of values compared, there are 10 deviations which exceed the magnitude of 0.03 rydberg, 31 deviations in the range 0.02-0.03 rydbergs and 162 deviations in the range 0.01-0.02 rydbergs. The remaining 331 computed band energies all lie within 0.01 rydberg of the reference energies. The largest deviation, in the value of 0.0742 rydberg, occurs for the 6^{th} band at $\vec{k} = (381)$. The direction $\vec{k} = (343)$ is the direction in the Brillouin zone along which the fitting is worst. Generally speaking, the fitting is worse for the higher bands. For the 1^{st} band, there are only 29 $\vec{k}$-vectors for which the deviation exceeds 0.01 rydberg whereas there are 45 $\vec{k}$-vectors for the 2^{nd} band, 49 $\vec{k}$-vectors for the 3^{rd} band, and 23, 16, 41 $\vec{k}$-vectors for the 4^{th}, 5^{th}, and 6^{th} bands respectively.

As indicated previously, the overall rms deviation for the 534 pairs of values is 0.18 eV (0.013 rydberg). This compares with the rms deviation of 0.11 eV[11] for Hodges' fitting of the same reference band structure with his interpolation scheme which did not incorporate the orthogonalization effects and with the rms deviation of less than 0.1 eV[12] for Mueller's fitting.

To have a better understanding of the importance of the inclusion of the orthogonalization effects as done by Mueller, we use our program to compute the interpolated band structure by leaving the orthogonalization effects out through setting the parameters B_4 and B_5 to zero. The results are referred to as those for the "Hodges' scheme" in our work and they are shown in Table 4-4. They are also shown in Fig.4-2 where the reference bands are also displayed. Comparing Fig. 4-1 and Fig. 4-2, it can be seen that the inclusion of orthogonalization effects in the so-called "hybrid scheme" produces a somewhat better fitting, particularly along Δ and Σ. However, the improvement is not dramatic. This is partly because the Hodges scheme automatically gives some allowance for orthogonalization effects through making α an adjustable parameter, as discussed in Chapter II Section 4 . The values of the interpolation parameters obtained for this "Hodges' scheme" and our "hybrid scheme" are also displayed side-by-side in Table 4-2. It may be noted that the parameters involving only d bands; namely E_0, Δ, $A_1, \ldots, A_6$, are identical in the two schemes. β is the bottom of the conduction band in both schemes. In the hybrid scheme, $\alpha = \frac{\hbar^2}{2m}\left(\frac{\pi}{4a}\right)^2 = 0.01322$, whereas, when allowing α to be adjustable as in Hodges' scheme, we have $\alpha = 0.01540$. The values of the pseudopotential parameters, V_{111} and V_{200} are, of course, greatly influenced by the inclusion of the orthogonalization effects, whereas the hybridization parameters R_1, K_2 and K_3 are much less affected. The orthogonalization parameters R_0 and K_0, of course, do not appear in Hodges' scheme.

In Table 4-6, we list the Burdick APW band values and interpolated band values as computed by Mueller[12], Hodges[11] and the scheme of the present work (labelled "Hybrid").
Rms deviations of these computed values from the Burdick values are also shown as the last line in the tabulation. Values used

for fitting in the Hodges scheme and the "Hybrid" scheme were not included in the computation of the rms deviation. It can be seen that the "Hybrid" scheme, with an rms deviation of 0.008 rydberg from the reference band structure, is somewhat superior to the Hodges scheme with an rms deviation of 0.015 rydberg.

As for ease of computation, it may be pointed out that instead of a fairly complicated and time consuming least-squares fitting for the interpolation parameters employed by Mueller[12], the algebriac expressions (3.9) and (3.101) allow the parameters to be fitted exactly. The computer time required for our explicit fitting is less than 1 minute. The entire computation, starting from the fitting of parameters, going through the setting up of the Hamiltonian matrix and its diagonalization and ordering the eigenvalues to the point where the eigenvalues and eigenvectors are ready for output, takes approximately 9 minutes for the execution time on an IBM-360 computer having a total core storage of 246,000 bytes. This time is sufficient for the computation of the 17 interpolation parameters and 9 band energy eigenvalues at 89 points in the Brillouin zone. Compilation time for the FORTRAN IV source program takes approximately 18 minutes on the same computer, with input in the form of punch cards. Output is available both on tape and paper print out.

4 Conclusion

In the present work, we have succeeded in working out the full details of a modified interpolation scheme for the paramagnetic band structures of transition metals and to give a full demonstration of the effectiveness and efficiency of the scheme with the example of Cu. The modified scheme combined the features developed by Hodges[11] for accounting for the tigh-binding d bands, the itinerant (pseudopotential) conduction bands, and the hybridization of the d and conduction bands with the features developed by Mueller[12] for accounting for the fairly important orthogonalization effects. We therefore referred to the new modified scheme as the "hybrid" scheme.

We also worked out an algebraic scheme for fitting all interpolation parameters from accurately calculated eigenvalues explicitly and exactly. All parameters are explicitly extracted including the parameters for describing the tigh-binding d-bands, the parameters for describing the itinerant (OPW) bands, the parameters describing the hybridization of the d-bands with the conduction bands and the orthogonalization effects of the two sets of bands.

A computer program was set up to perform the entire computation starting from the parameter fitting, going through the setting up of the hamiltonian matrix and its diagonalization to yield eigenvalues and eigenvectors for each reciprocal lattice vector in the Brillouin zone. It was employed to compute the paramagnetic band structure of Cu using APW band energies at high symmetry points in the Brillouin zone computed by Burdick for fixing the interpolation parameters.

The hybrid scheme was found to be very successful in reproducing the reference band structure. For the lowest six bands at 89 points in the Brillouin zone of Cu, an rms deviation of 0.18 eV is obtained. The largest deviation is 0.0742 rydberg and it occurs at $\vec{k}$ = (381). The hybrid scheme is found to be somewhat superior to the original scheme of Hodges in precision and to the scheme of Mueller in both precision and ease of computation.

APPENDICES

Appendix A

Symmetrized Plane Waves

This appendix is taken from Ref. 10. The combinations of plane waves appearing in the Bloch eigenfunctions are expressed in terms of the reciprocal lattice vectors $\vec{K}_1,\ldots,\vec{K}_4$ as defined in (2.18). The coefficients $c_1,\ldots,c_4$ of the properly symmetrized plane waves at high symmetry points in the 1/48 of the Brillouin zone as listed in the table below are in the forms:

$$c_1 e^{i(\vec{k}+\vec{K}_1)\cdot\vec{r}} + c_2 e^{i(\vec{k}+\vec{K}_2)\cdot\vec{r}} + c_3 e^{i(\vec{k}+\vec{K}_3)\cdot\vec{r}} + c_4 e^{i(\vec{k}+\vec{K}_4)\cdot\vec{r}}$$

POINT	LEVEL	c_1	c_2	c_3	c_4
(0,0,0)	Γ_1	1	0	0	0
(0,π,0)	X_1	$1/\sqrt{2}$	$1/\sqrt{2}$	0	0
	$X_{4'}$	$1/\sqrt{2}$	$-1/\sqrt{2}$	0	0
$\left(\frac{\pi}{2},\frac{\pi}{2},\frac{\pi}{2}\right)$	L_1	$1/\sqrt{2}$	0	$1/\sqrt{2}$	0
	$L_{2'}$	$1/\sqrt{2}$	0	$-1/\sqrt{2}$	0
$\left(\frac{3\pi}{4},\frac{3\pi}{4},0\right)$	K_1	1	0	0	0
	K_1	0	0	$1/\sqrt{2}$	$1/\sqrt{2}$
	K_3	0	0	$1/\sqrt{2}$	$-1/\sqrt{2}$

POINT	LEVEL	c_1	c_2	c_3	c_4
$\left(\frac{\pi}{2},\pi,0\right)$	W_1	1/2	-1/2	1/2	-1/2
		1/2	-1/2	-1/2	1/2
	W_1	1/2	1/2	1/2	1/2
	$W_{2'}$	1/2	1/2	-1/2	-1/2

Appendix B

Symmetrized LCAO's

This appendix is taken from Ref. 10 . The properly symmetrized combinations of atomic orbitals corresponding to different irreducible representations S_i at various symmetry points in the 1/48 of the Brillouin zone used in the present calculations are given in the form:

$$b_{S_i}(\vec{k},\vec{r}) = N^{-1} \sum_{\ell} e^{i\vec{k}\cdot\vec{R}_\ell} \varphi_{S_i}(\vec{r}-\vec{R}) .$$

The table below lists the φ_{S_i} at various symmetry points, which are expressed in terms of the $\varphi_n(\vec{r})$ as given in (2.11), (2.11A) and (2.11B). All the positions in the Brillouin zone are expressed in terms of $(\xi,\eta,\zeta) = \frac{1}{2}a(k_x,k_y,k_z)$.

POINT	LEVEL	φ_{S_i}
(0,0,0)	$\Gamma_{25'}$	$\varphi_1 \sim xy$
		$\varphi_2 \sim yz$
		$\varphi_3 \sim zx$
	Γ_{12}	$\varphi_4 \sim \frac{1}{2}(x^2-y^2)$
		$\varphi_5 \sim \frac{1}{2\sqrt{3}}(2z^2-x^2-y^2)$

POINT	LEVEL	φ_{S_i}
$(0,\pi,0)$	X_5	$\begin{cases}\varphi_1\\ \varphi_2\end{cases}$
	X_3	φ_3
	X_2	$\frac{1}{2}(\varphi_4-\sqrt{3}\,\varphi_5) \sim \frac{1}{2}(x^2-z^2)$
	X_1	$\frac{1}{2}(\sqrt{3}\,\varphi_4+\varphi_5) \sim \frac{1}{2\sqrt{3}}(x^2+z^2-2y^2)$
$\left(\frac{\pi}{2},\frac{\pi}{2},\frac{\pi}{2}\right)$	L_1	$\frac{1}{\sqrt{3}}(\varphi_1+\varphi_2+\varphi_3) \sim \frac{1}{\sqrt{3}}(xy+yz+zx)$
	L_3	$\begin{cases}\frac{1}{\sqrt{2}}(\varphi_1-\varphi_3) \sim \frac{1}{\sqrt{2}}(xy-zx)\\ \frac{1}{\sqrt{6}}(\varphi_1-2\varphi_2+\varphi_3) \sim \frac{1}{\sqrt{6}}(xy-2yx+zx)\end{cases}$
	L_3	$\begin{cases}\frac{1}{2}(\varphi_4+\sqrt{3}\,\varphi_5) \sim \frac{1}{2}(z^2-y^2)\\ \frac{1}{\sqrt{2}}(\sqrt{3}\,\varphi_4-\varphi_5) \sim \frac{1}{2\sqrt{3}}(2x^2-y^2-z^2)\end{cases}$
$\left(\frac{3\pi}{4},\frac{3\pi}{4},0\right)$	K_4	φ_4
$\left(\frac{\pi}{2},\pi,0\right)$	$W_{2'}$	$\frac{1}{2}(\varphi_4+\sqrt{3}\,\varphi_5) \sim \frac{1}{2}(z^2-y^2)$
	W_1	$\frac{1}{2}(\sqrt{3}\,\varphi_4-\varphi_5)$
	W_3	$\begin{cases}\varphi_1\\ \varphi_3\end{cases}$

Appendix C

FORTRAN IV Program for a Hybrid Interpolation Scheme

The 17 interpolation parameters are denoted by the following expressions in the FORTRAN program.

Parameter	Expressions in Program
E_o	E
Δ	DELTA
A_1	A1
A_2	A2
A_3	A3
A_4	A4
A_5	A5
A_6	A6
α	ALPHA
β	BETA
V_1	V1
V_2	V2

Parameter	Expressions in Program
B_1	B1
B_2	B2
B_3	B3
B_4	B4
B_5	B5

The other quantities which appear in the source program are denoted as follows:

$$F_{000}(\vec{k}) \longrightarrow C1$$

$$F_{0\bar{2}0}(k) \longrightarrow C2$$

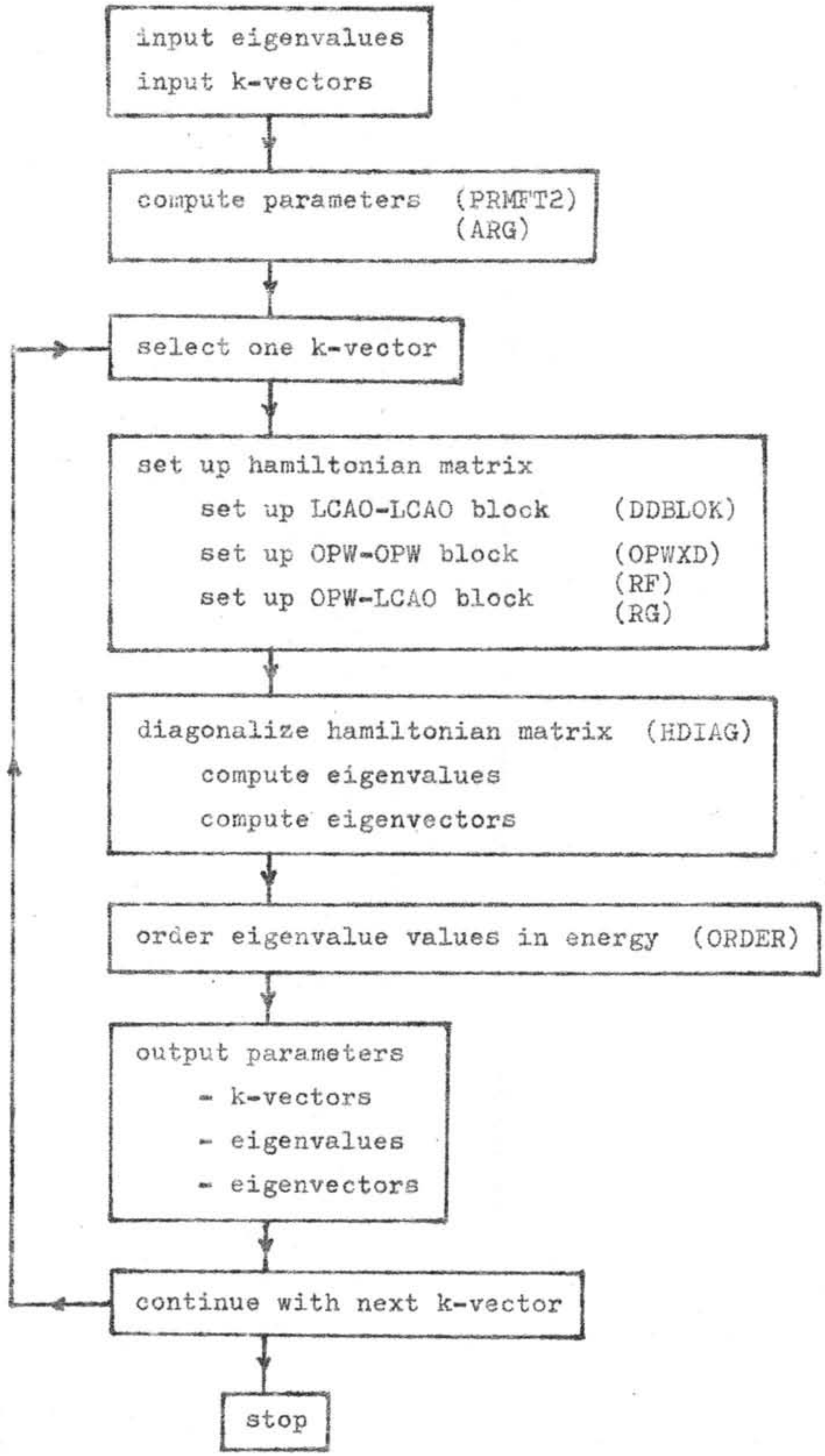
$$F_{\bar{1}\bar{1}\bar{1}}(\vec{k}) \longrightarrow C3$$

$$F_{\bar{1}\bar{1}1}(\vec{k}) \longrightarrow C4$$

$$j_2(Y) \longrightarrow BJ2(Y)$$

A flow-chart indicating the major action step of the program and the source program used in our present work are shown below.

Flow-chart of the computer program



The Source Program

The main program

```
C     INTERPOLATION SCHEME FOR PARAMAGNETIC COPPER BAND STRUCTURE
     ODIMENSION W(90), X(90), Y(90), Z(90), H(9,9), U(9,9),
     1XXXX(9), IQ(9)
      DIMENSION III(9)
      DIMENSION HH(9)
      DIMENSION UU(9,9)
      DIMENSION CE(17),II(17)
      COMMON /PARAM/ A1,A2,A3,A4,A5,A6,E,DELTA,V1,V2,ALPHA,BETA1,
     1BETA2,B1,B2,B3,B4,B5
      COMMON H
      DATA II/3,2,1,14,5,4,6,7,8,9,10,11,13,12,15,16,17/
      NAMELIST
C     DEFINITION OF SPHERICAL BESSEL FUNCTION OF ORDER TWO, WHICH
C             APPEARS IN THE HYBRIDIZATION MATRIX ELEMENTS.
      WRITE (6,125)
125   FORMAT (1H1)
C        SET METHOD=1 IF PARAMETERS ARE TO BE INPUT.
C        SET METHOD=2 IF EIGENVALUES ARE TO BE INPUT AND THE
              PARAMETERS CALCULATED FROM THEM.
C        INPUT METHOD
      READ(5,90) METHOD
90    FORMAT(1X,I1)
      WRITE(6,91) METHOD
91    FORMAT(3X,8HMETHOD =,I2)
      READ(5,115) RAP,IEIGEN,IHAMIL,IVECTR,NPTS
115   FORMAT(E14.0,4I3)
      READ(5,150) (W(I),X(I),Y(I),Z(I),I=1,NPTS)
150   FORMAT( 5(1X,F2.0,3F3.2))
      GO TO (101,102),METHOD
101   CONTINUE
      READ(5,110) A1,A2,A3,A4,A5,A6,E,DELTA
      READ(5,110) V1,V2,ALPHA,BETA1,BETA2,B1,B2,B3
      READ(5,110) B4,B5
110   FORMAT (2X, 8F8.5)
      GO TO 105
102   CONTINUE
C        N IS THE NUMBER OF SYMMETRY PT. E.V.'S TO BE READ IN
C        IEQ = 0 : B2=B3,         B4,B5 : ZERO
C        IEQ = 1 : B2.NE.B3,      B4,B5 : ZERO
C        IEQ = 2 : B2=B3,         B4,B5 : NONZERO
C        IEQ = 3 : B2.NE.B3,      B4,B5 : NONZERO
C        CURRENT PROGRAM CANNOT ACCEPT IEQ = 1,2
      READ(5,2002) N,IEQ
2002  FORMAT(I2,7X,I1)
      WRITE(6,70) IEQ
70    FORMAT(3X,5HIEQ =,I2//)
C        ORDER OF INPUT USING READ CE(II(I)):
C          G1,G25',G12,X11,X3,X2,X5,
C          X4',K4,L11,L31,L32,L12,L2',X11,
C          W21,X12,W22.
C        ORDER OF ELEMENTS OF ARRAY CE (CALCULATED ENERGIES)
```

```
C          G12,G25',G1,X2,X3,X5,X4',
C          K4,L11,L31,L32,L12,L2',X11,
C          W21,X12,W22.
      READ(5,2000) (CE(II(I)),I=1,N)
2000  FORMAT(7(F9.6))
      WRITE(6,2001)(CE(II(I)),I=1,N)
2001  FORMAT(3(1X,7(F9.5)/))
      WRITE(6,2003)
2003  FORMAT(//)
C        A IS LATTICE CONSTANT
C        INPUT A
      READ(5,60) A
60    FORMAT(F8.5)
      WRITE(6,50) A
50    FORMAT(3X,3HA =,F9.5//)
      CALL PRMFT2(A,CE,IEQ)
105   CONTINUE
C        SET IEIGEN=0 IF EIGENVALUE PRINTOUT ISN'T DESIRED.
C        SET IEIGEN=2 IF EIGENVALUE PRINTOUT AT 89 POINTS IS DESIRED.
C        SET IHAMIL=0 IF HAMILTONIAN MATRIX ISN'T DESIRED IN PRINTOUT.
C        SET IVECTR=0 IF EIGENVECTOR PRINTOUT ISN'T DESIRED.
C        OTHERWISE SET THESE INTEGERS EQUAL TO 1.
      IEIGEN=2
      RAP=1.E-04
      WRITE(6,135) A1,A2,A3,A4,A5,A6,E,DELTA
      WRITE(6,135) V1,V2,ALPHA,BETA1,BETA2,B1,B2,B3
      WRITE(6,135) B4,B5
135   FORMAT(3X, 8F10.5)
      WRITE(6,140) NPTS
140   FORMAT(3X, I4)
      WRITE(6,145) RAP
145   FORMAT(6HORAP =,1PE15.8)
C        ISYM = 1 N. SMITH SYMMETRIZATION
C        ISYM = 0 NO SYMMETRIZATION
C        INPUT ISYM
      READ(5,30) ISYM
30    FORMAT(1X,I1)
      WRITE(6,20) ISYM
20    FORMAT(3X,6HISYM =,I2//)
200   DO 450 I=1,NPTS
      WW=W(I)
      XX=X(I)
      YY=Y(I)
      ZZ=Z(I)
C
      CALL DDBLOK(XX,YY,ZZ)
C        THIS GIVES D-D BLOCK OF HAMILTONIAN MATRIX.
      CALL OPWXD(XX,YY,ZZ,ISYM,IEQ)
C        THIS GIVES OPW-OPW AND OPW-D BLOCKS OF HAMILTONIAN MATRIX.
C
300   IF (IHAMIL) 301, 321,301
```

```
C     HAMILTONIAN MATRIX IS MADE SYMMETRIC FOR EASE IN READING
C            IT IN ITS PRINTED FORM.
301   DO 310 L=1,9
      DO 310 K=L,9
310   H(K,L)=H(L,K)
      WRITE(6,318)
      WRITE(6,318)
318   FORMAT(//)
319   WRITE(6,320) ((H(M,N), M=1,9), N=1,9)
320   FORMAT (9(3X,F10.6))
C     DIAGONALIZE THE NAMILTONIAN MATRIX.
321   N=9
      IEGEN=0
      NR=0
      CALL HDIAG(H,N,IEGEN,U,NR,XXXX,IQ,RAP)
      IF (IEIGEN) 323,335,323
323   CONTINUE
      IF(IEIGEN.EQ.2.AND.ABS(INT(XX)+INT(YY)+INT(ZZ)-XX-YY-ZZ).GT.
     13.E-06) GO TO 335
326   HH(J)=H(J,J)
      CALL ORDER(HH,III,9)
      DO 327 J=1,9
327   H(J,J)=H(J)
      DO 328 J=1,9
      DO 328 K=1,9
328   UU(J,K)=U(J,K)
      DO 329 K=1,9
      DO 329 J=1,9
329   U(J,K)=UU(J,III(K))
      WRITE(6,324) XX,YY,ZZ,WW,(H(J,J),J=1,9)
324   FORMAT(1X,'(',2(F4.2,','),F4.2,')',3X,F5.2,4X,9(1X,F10.4))
335   CONTINUE
400   IF (IVECTR) 401, 450, 401
401   DO 410 M=1,9
      DO 410 N=1,9
410   U(M,N)=U(M,N)*ABS(U(M,N)*WW
      WRITE(6,420)((U(M,N),N=1,9),M=1,9)
420   FORMAT(//9(3X,F10.4))
450   CONTINUE
580   WRITE(6,590)
590   FORMAT (14HOJOB COMPLETED)
600   STOP
      END
```

The subroutines

```
      SUBROUTINE PRMFT2(A,CE,IEQ)
C        A IS LATTICE CONSTANT
C        IEQ = 0 : B2=B3    ,    B4,B5 : ZERO
C        IEQ = 1 : B2.NE.B3,    B4,B5 : ZERO
C        IEQ = 2 : B2=B3    ,    B4,B5 : NONZERO
C        IEQ = 3 : B2.NE.B3,    B4,B5 : NONZERO
C        CURRENT PROGRAM CANNOT ACCEPT IEQ = 1,2
      DIMENSION CE(17)
      COMMON /PARAM/ A1,A2,A3,A4,A5,A6,E,DELTA,V1,V2,ALPHA,
     1BETA1,BETA2,B1,B2,B3,B4,B5
      REAL KX,KL,KW
      REAL LA,LB,LC
      REAL NXS,NXD,NLS,NLD
      BJ2(Y)=((3.0-Y*Y)*SIN(Y)-3.0*Y*COS(Y))/(Y*Y*Y)
      GAMMA(E1,E2,ED)=SQRT((E2-ED)*(ED-E1))
      A1=(CE(6)+CE(6)-CE(2)-CE(5))/16.0
      A2=(CE(2)-CE(5))/16.0
      A5=(CE(4)-CE(1))/16.0
      A4=(CE(1)-CE(8))/2.0+(4.0+SQRT(8.0))*A5
      E=(CE(6)+CE(6)+CE(2)+CE(5))/4.0
      DELTA=CE(1)-E+8.0*A5-4.0*A4
      A3=(CE(10)-E+CE(11)-E-DELTA)/4.0
      A6=SQRT(((CE(10)-CE(11))**2-(DELTA-4.0*A3)**2)/128.0)
      BETA1=CE(3)
      BETA2=0.0
      BETA=BETA1
      PI=3.1415926536
      ALPHA=((2.*PI/A)**2)/64.0
      SX=BETA+64.* ALPHA
      SL=BETA+48.* ALPHA
      SW=BETA+80.* ALPHA
      DX1=E+DELTA-(20./3.)*A4-(8./3.)*A5
      DL1=E-8.*A3
      DW2=E+DELTA-4.*A4
      DW1=E+DELTA+(4./3.)*A4+(16./3.)*A5
      EXS=CE(16)+CE(14)
      EXD=CE(16)-CE(14)
      EX=CE(14)+CE(16)+CE(7)
      ELS=CE(12)+CE(9)
      ELD=CE(12)-CE(9)
      EL=CE(9)+CE(12)+CE(13)
      KX=8.0
      KL=SQRT(48.0)
      KW=SQRT(80.0)
      GX1=GAMMA(CE(14),CE(16),DX1)
      GL1=GAMMA(CE(9),CE(12),DL1)
      GW2=GAMMA(CE(15),CE(17),DW2)
      IF (IEQ.EQ.0) GO TO 5
      RATIO1=SQRT(24./25.)*GX1/GW2
      CALL ARG(RATIO1,KX,KW,XX)
      GO TO 6
```

```
5     RATIO1=GX1/GL1
      CALL ARG(RATIO1,KX,KL,XX)
6     IF (XX.LT.0) GO TO 7
      B1=XX
      HJ2X=BJ2(KX*B1)
      HJ2L=BJ2(KL*B1)
      HJ2W=BJ2(KW*B1)
      B2=SQRT(1.5)*GL1/HJ2L
      B3X=SQRT(1.5)*GX1/HJ2X
      B3W=1.25*GW2/HJ2W
C     OUTPUT B3X,B3W
      B3=B3X
      IF (IEQ.EQ.0) B3=B2
      GO TO 8
7     B1=1.0
      B2=0.0
      B3=0.0
C     OUTPUT 'ERROR : NEGATIVE B1'
      STOP 222
8.    CONTINUE
      IF (IEQ.EQ.0) GO TO 9
      XIX=B3*BJ2(KX*B1)
      XIL=B2*BJ2(KL*B1)
      XIXSQ=XIX*XIX
      XILSQ=XIL*XIL
      AX=2.*SX+DX1-EX
      BX=EX/3.-DX1
      AL=2.*SL+DL1-EL
      BL=EL/3.-DL1
      XA=BX*BX+16.*XIXSQ/27.
      XB=2.*AX*BX-16.*XIXSQ/9.
      XC=AX*AX
      LA=BL*BL+16.*XILSQ/27.
      LB=2.*AL*BL-16.*XILSQ/9.
      LC=AL*AL
      RX2=XB*XB-4.*XA*XC
      RL2=LB*LB-4.*LA*LC
      DISCX=SQRT(RX2)
      DISCL=SQRT(RL2)
      ETAXD=(-XB-DISCX)/(2.*XA)
      ETALD=(-LB-DISCL)/(2.*LA)
      ZETAXD=SQRT(ETAXD)
      ZETALD=SQRT(ETALD)
      RATIOD=ZETAXD/ZETALD
      CALL ARG(RATIOD,KX,KL,B4D)
      B4=B4D
      OJ2XD=BJ2(KX*B4D)
      OJ2LD=BJ2(KL*B4D)
      B5XD=ZETAXD/OJ2XD
      B5LD=ZETALD/OJ2LD
      B5=B5XD
```

```
      CXD=1.-(1./3.)*ETAXD
      CLD=1.-(1./3.)*ETALD
      GO TO 10
9     B4=0.0
      B5=0.0
      CXD=1.0
      CLD=1.0
10    CONTINUE
      V2D=SX-CE(7)*CXD
      V1D=SL-CE(13)*CLD
      V1=V1D
      V2=V2D
      RETURN
      END
```

```
      SUBROUTINE ARG(R,C1,C2,X)
      BJ2(Y)=((3.0-Y*Y)*SIN(Y)-3.0*Y*COS(Y))/(Y*Y*Y)
      X=0.05
      DELTAX=0.1
      N=0
      ERROR1=R-BJ2(C1*X)/BJ2(C2*X)
1     CONTINUE
      N=N+1
      IF (N.GT.200) GO TO 4
      X=X+DELTAX
      RATIO=BJ2(C1*X)/BJ2(C2*X)
      ERROR2=R-RATIO
      IF (ERROR1*ERROR2.GT.0.0) GO TO 2
      IF (DELTAX.LT.1.0E-06) GO TO 3
      DELTAX=0.6*DELTAX
      X=X-DELTAX-DELTAX
      ERROR2=ERROR1
2     ERROR1=ERROR2
      GO TO 1
3     CONTINUE
      RETURN
C     OUTPUT 'ERROR : NO CONVERGENCE IN SUBROUTINE ARG' R,C1,C2
4     STOP 333
5     X=-1.0
      RETURN
      END
```

```
      SUBROUTINE DDBLOK(XX,YY,ZZ)
C        CALCULATES D-D BLOCK, FROM HODGES
      DIMENSION H(9,9)
      COMMON /PARAM/ A1,^2,A3,A4,A5,A6,E,DELTA,V1,V2,ALPHA,
     1BETA1,BETA2,B1,B2,B3,B4,B5
      COMMON H
      PI=3.1415926536
      X1=PI*XX/8.0
      Y1=PI*YY/8.0
      Z1=PI*ZZ/8.0
      XYZ=XX+YY+ZZ
      XY=XX+YY
      CAX=COS(PI*XX/12.0)
      CIX=COS(X1)
      CIY=COS(Y1)
      CIZ=COS(Z1)
      SIX=SIN(X1)
      SIY=SIN(Y1)
      SIZ=SIN(Z1)
      H(5,5)=-4.*A1*CIX*CIY+4.*A2*CIZ *(CIX+CIY)+1.0+E
      H(5,6)=-4. *A3*SIX*SIZ
      H(5,7)=-4.*A3*SIY*SIZ
      H(5,8)=0.00
      H(5,9)=-(8./1.73205)*A6*SIX*SIY
      H(6,6)=-4.*A1*CIY*CIZ+4.* A2*CIX* (CIY+CIZ)+1.0+E
      H(6,7)=-4.*A3 *SIX* SIY
      H(6,8)=-4. *A6*SIY*SIZ
      H(6,9)=+(4./1.73205)*A6* SIY*SIZ
      H(7,7)=-4.*A1*CIX*CIZ+4.*A2*CIY* (CIX+CIZ)+1.0+E
      H(7,8)=+4.*A6*SIX*SIZ
      H(7,9)=+(4./1.73205)* A6* SIX*SIZ
      H(8,8)=+4.*A4*CIX*CIY-4. *A5*CIZ *(CIX+CIY)+1.0+E+DELTA
      H(8,9)=+(4./1.73205) *(A4+A5)*CIZ *(CIY-CIX)
     0H(9,9)=-(4./3.)*(A4+4.* A5) *CIX*CIY+(4./3.)*(2.*A4-A5)*
     1CIZ*(CIX+CIY)+1.0+E+DELTA
      DO 2 I=5,9
2     H(I,I)=H(I,I)-1.0
      DO 1 I=5,9
      DO 1 J=I,9
1     H(J,I)=H(I,J)
      RETURN
      END
```

```
      SUBROUTINE OPWXD(XX,YY,ZZ,ISYM,IEQ)
C        BASED ON F.M. MUELLER SUBROUTINE HSOC PROGRAM QUAD
C        CALCULATES OPW-OPW BLOCK AND OPW-D INTERACTION BLOCK
C        ISYM = 1  N. SMITH SYMMETRIZATION
C        ISYM = 0  NO SYMMETRIZATION
      DIMENSION H(9,9)
      DIMENSION AK(4,3),BK(3),ES(9,9),GF(4),GN(4),CK(3),GG(4,9)
      DIMENSION CC(4)
      COMMON /PARAM/ A1,A2,A3,A4,A5,A6,E,DELTA,V1,V2,ALPHA,
     1BETA1,BETA2,B1,B2,B3,B4,B5
      COMMON H
      PI=3.1415926536
      AK(1,1)=0.0
      AK(1,2)=0.0
      AK(1,3)=0.0
      AK(2,1)=0.0
      AK(2,2)=-16.0
      AK(2,3)=0.0
      AK(3,1)=-8.0
      AK(3,2)=-8.0
      AK(3,3)=-8.0
      AK(4,1)=-8.0
      AK(4,2)=-8.0
      AK(4,3)=8.0
C     COMPUTE THE SYMMETRIZING FACTORS C2, C3, C4.
      DO 5 I=1,4
5     CC(I)=1.
      IF(ISYM.EQ.0) GO TO 12
      C1=1.0
      C2=(SIN(PI*(YY-XX)/(2.0*(16.0-XX-YY))))**2
      C3=(SIN(PI*(XX+ZZ)/(2.0*(12.0-YY))))**2
      C4=(SIN(PI*(XX-ZZ)/(12.0-YY)/2.0))**2
      CC(1)=C1
      CC(2)=C2
      CC(3)=C3
      CC(4)=C4
12    CONTINUE
      DO 2 I=1,4
      BK(1)=XX
      BK(2)=YY
      BK(3)=ZZ
      GO=0.0
      DO 3 J=1,3
      CK(J)=AK(I,J)+BK(J)
3     GO=GO+CK(J)*CK(J)
      GI=SQRT(GO)
      ITEST=1
      TEST=ABS(GI)
      BEST=10.E-20
      IF (TEST.GE.BEST) GO TO 94
      GI=1.0
```

```
      ITEST=0
94    CONTINUE
      A=CK(1)/GI
      B=CK(2)/GI
      C=CK(3)/GI
      ES(5,I)=A*B
      ES(6,I)=B*C
      ES(7,I)=C*A
      ES(8,I)=.5*(A*A-B*B)
      ES(9,I)=.5*SQRT(1./3.)*(3.*C*C-1.)
      IF (ITEST) 95, 96, 95
96    GI=0.0
95    CONTINUE
      IF(IEQ.EQ.0) B3=B2
      CALL RG(GI,Z2,B2,B1)
      CALL RG(GI,Z3,B3,B1)
      DO 90 J=5,7
90    GG(I,J)=Z2
      DO 85 J=8,9
85    GG(I,J)=Z3
      DO 50 J=5,9
50    H(I,J)=ES(J,I)*CC(I)*GG(I,J)
      CALL RF(GI,Z,B5,B4)
      GF(I)=Z
      GN(I)=SQRT(1.-GF(I)*GF(I)/3.)
2     H(I,I)=GO*ALPHA*BETA1
      H(1,2)=V2*CC(2)
      H(1,3)=V1*CC(3)
      H(1,4)=V1*CC(4)
      H(2,3)=V1*SQRT(CC(2)*CC(3))
      H(2,4)=V1*SQRT(CC(2)*CC(4))
      H(3,4)=V2*SQRT(CC(3)*CC(4))
      DO 10 I=1,4
      DO 10 J=I,4
      SUM=0.0
      SIMI=0.0
      SIMJ=0.0
      DO 11 K=5,9
      SIMI=SIMI+ES(K,I)*ES(K,J)*GG(I,K)
      SIMJ=SIMJ+ES(K,I)*ES(K,J)*GG(J,K)
      DO 11 L=5,9
      A=H(K,L)
11    SUM=SUM+ES(K,I)*ES(L,J)*A
      H(I,J)=H(I,J)-SUM*GF(I)*GF(J)+(SIMI*GN(I)*GF(J)+SIMJ*GN(J)*
     1GF(I))
10    H(I,J)=H(I,J)/(GN(I)*GN(J))
      RETURN
      END
```

```
      SUBROUTINE RG(GI,Z,T,RR)
C        CALCULATES HYBRIDIZATION FORM FACTOR
      C=T
      A=GI*RR
      IF (A-1.E-02) 22, 22, 8
8     CONTINUE
      IF (A-4.25) 20, 20, 10
10    IF (A-5.1)  16, 15, 15
15    Z=0.0
      RETURN
16    C=T*(5.1-A)/.85
20    Z=(3./A** 3-1./A)* SIN(A)-3.* COS(A)/A** 2
      Z=Z*C
      RETURN
22    Z=(A**2)/15.-(A**4)/210.
      Z=Z*C
      RETURN
      END
```

```
      SUBROUTINE RF(GI,Z,T,RR)
C        CALCULATES OVERLAP FORM FACTOR
31    A=GI*RR
      IF (A-1.E-02) 33, 33, 311
311   IF (A-5.8) 3, 3, 32
3     Z=(3./A**3-1./A)*SIN(A)-3.*COS(A)/A**2
      Z=T*ABS(Z)
      GO TO 16
32    Z=0.0
      RETURN
33    Z=(A**2)/15.-(A**4)/210.
      Z=T*ABS(Z)
16    RETURN
      END
```

```
      SUBROUTINE HDIAG(H,N,IEGEN,U,NR,X,IQ,RAP)
C     FORTRAN IV DIAGONALIZATION OF A SYMMETRIC REAL MATRIX BY
C           JACOBI METHOD WHERE H IS THE ARRAY TO BE
C           DIAGONALIZED.
C     N IS THE ORDER OF THE MATRIX, H.
C     IEGEN MUST BE SET UNEQUAL TO ZERO IF ONLY EIGENVALUES
C           ARE TO BE COMPUTED.
C     IEGEN MUST BE SET EQUAL TO ZERO IF EIGENVALUES AND
C           EIGENVECTORS ARE TO BE COMPUTED.
C     U IS THE UNITARY MATRIX USED FOR FORMATION OF THE
C           EIGENVECTORS.
C     NR IS THE NUMBER OF ROTATIONS.
C     THE SUBROUTINE OPERATES ONLY ON THE ELEMENTS OF H THAT ARE
C           TO THE RIGHT OF THE MAIN DIAGONAL.  THUS, ONLY A
C           TRIANGULAR SECTION NEED BE STORED IN THE
C           ARRAY H.
      DIMENSION H(9,9),U(9,9),X(9),IQ(9)
      IF (IEGEN)  15,10,15
10    DO 14 I=1,N
      DO 14 J=1,N
      IF (I-J)  11,12,11
11    U(I,J) = 0.0
      GO TO 14
12    U(I,I) = 1.0
14    CONTINUE
15    NR = 0
      IF (N-1)   1000, 1000, 17
C     SCAN FOR LARGEST OFF DIAGONAL ELEMENT IN EACH ROW.
C     X(I) CONTAINS LARGEST ELEMENT IN ITH ROW.
C     IQ(I) HOLDS SECOND SUBSCRIPT DEFINING POSITION OF ELEMENT.
17    NMI1 = N-1
      DO 30 I=1.NMI1
      X(I) = 0.0
      IPL1 = I+1
      DO 30 J = IPL1,N
      SET = ABS(H(I,J))
      IF (X(I)-SET) 20, 20, 30
20    X(I) = SET
      IQ(I) = J
30    CONTINUE
      HDTEST = 1.0E38
C     FIND MAXIMUM OF X(I)'S FOR PIVOT ELEMENT AND TEST FOR END
C           OF PROBLEM.
40    DO 70 I = 1, NMI1
      IF (I-1) 60, 60, 45
45    IF (XMAX-X(I)) 60, 70, 70
60    XMAX = X(I)
      IPIV = I
      JPIV = IQ(I)
70    CONTINUE
```

```
C     IF MAX. X(I) EQUAL TO ZERO, IF LESS THAN HDTEST,
C            REVISE HDTEST.
      IF (XMAX) 1000, 1000, 80
80    IF (HDTEST) 90, 90, 85
85    IF (XMAX-HDTEST) 90, 90, 148
90    HDIMIN = ABS(H(1,1))
      DO 110 I = 2,N
      PUT = ABS(H(I,I))
      IF (HDIMIN-PUT) 110, 110, 100
100   HDIMIN = PUT
110   CONTINUE
      HDTEST = HDIMIN*RAP
C     RETURN IF MAX. H(I,J) LESS THAN RAP*ABS(H(K,K)-MIN)
      IF (HDTEST-XMAX) 148, 1000, 1000
148   NR =NR+1
C     COMPUTE TANGENT, SINE AND COSINE OF H(I,I) AND H(J,J).
150   OTANG=SIGN(2.0,(H(IPIV,IPIV)-H(JPIV,JPIV)))* H(IPIV,JPIV)
     1/(ABS(H(IPIV,IPIV)-H(JPIV,JPIV))+SQRT((H(IPIV,IPIV)-H(
     2JPIV,JPIV))**2+4.0*H(IPIV,JPIV)** 2))
      COSINE=1.0/SQRT(1.0+TANG**2)
      SINE=TANG *COSINE
      HII=H(IPIV,IPIV)
      H(IPIV,IPIV)=COSINE**2*(HII+TANG*(2.* H(IPIV,JPIV)+TANG*
     1H(JPIV,JPIV)))
      H(JPIV,JPIV)=COSINE**2*(H(JPIV,JPIV)-TANG *(2.*H(IPIV,JPIV)
     1-TANG*HII))
      H(IPIV,JPIV)=0.0
C     PSEUDO RANK THE EIGENVALUES
C     ADJUST SINE AND COS FOR COMPUTATION OF H(I,K) AND U(I,K).
      IF (H(IPIV,IPIV)-H(JPIV,JPIV)) 152, 153, 153
152   HTEMP=H(IPIV,IPIV)
      H(IPIV,IPIV)=H(JPIV,JPIV)
      H(JPIV,JPIV)=HTEMP
C     RECOMPUTE SINE AND COS
      HTEMP=SIGN(1.0,-SINE)* COSINE
      COSINE=ABS(SINE)
      SINE=HTEMP
153   CONTINUE
C     INSPECT THE IQ'S BETWEEN I+1 AND N-1 TO DETERMINE
C     WHETHER A NEW MAXIMUM VALUE SHOULD BE COMPUTED SINCE
C     THE PRESENT MAXIMUM IS IN THE I OR J ROW.
      DO 350 I=1,NMI1
      IF (I-IPIV) 210, 350, 200
200   IF (I-JPIV) 210, 350, 210
210   IF (IQ(I)-IPIV) 230, 240, 230
230   IF (IQ(I)-JPIV) 350, 240, 350
240   K=IQ(I)
250   HTEMP=H(I,K)
      H(I,K)=0.0
      IPL1=I+1
      X(I)=0.0
C     SEARCH IN DEPLETED ROW FOR NEW MAXIMUM.
```

```
      DO 320 J=IPL1,N
      SET =ABS(H(I,J))
      IF (X(I)-SET) 300, 300, 320
300   X(I)=SET
      IQ(I)=J
320   CONTINUE
      H(I,K)=HTEMP
350   CONTINUE
      X(IPIV)=0.0
      X(JPIV)=0.0
C     CHANGE THE OTHER ELEMENTS OF H
      DO 530 I=1,N
      IF (I-IPIV) 370, 530, 420
370   HTEMP=H(I,IPIV)
      H(I,IPIV)=COSINE*HTEMP+SINE*H(I,JPIV)
      SET=ABS(H(I,IPIV)
      IF (X(I)-SET) 380, 390, 390
380   X(I)=SET
      IQ(I)=IPIV
390   H(I,JPIV)=-SINE*HTEMP+COSINE*H(I,JPIV)
      PUT=ABS(H(I,JPIV))
      IF (X(I)-PUT) 400, 530, 530
400   X(I)=PUT
      IQ(I)=JPIV
      GO TO 530
420   IF (I-JPIV) 430, 530, 480
430   HTEMP=H(IPIV,I)
      H(IPIV,I)=COSINE*HTEMP+SINE*H(I,JPIV)
      PLACE=ABS(H(IPIV,I))
      IF (X(IPIV)-PLACE) 440, 450, 450
440   X(IPIV)=PLACE
      IQ(IPIV)=I
450   H(I,JPIV)=-SINE*HTEMP+COSINE*H(I,JPIV)
      PUT=ABS(H(I,JPIV))
      IF (X(I)-PUT) 400, 530, 530
480   HTEMP=H(IPIV,I)
      H(IPIV,I)=COSINE*HTEMP+SINE*H(JPIV,I)
      PLACE=ABS(H(IPIV,I))
      IF (X(IPIV)-PLACE) 490, 500, 500
490   X(IPIV)=PLACE
      IQ(IPIV)=I
500   H(JPIV,I)=-SINE*HTEMP+COSINE*H(JPIV,I)
      FIX=ABS(H(JPIV,I))
      IF (X(JPIV)-FIX) 510, 530, 530
510   X(JPIV)=FIX
      IQ(JPIV)=I
530   CONTINUE
C     TEST FOR COMPUTATION OF EIGENVECTORS
      IF (IEGEN) 40, 540, 40
540   DO 550 I=1,N
      HTEMP=U(I,IPIV)
```

```
      U(I,IPIV)=COSINE*HTEMP+SINE*U(I,JPIV)
550   U(I,JPIV)=-SINE*HTEMP+COSINE*U(I,JPIV)
      GO TO 40
1000  RETURN
      END
```

```
      SUBROUTINE ORDER(A,INDEX,N)
      DIMENSION A(N),INDEX(N)
      DO 4 I=1,N
4     INDEX(I)=I
      NN=N-1
      DO 2 J=1,NN
      IORDER=0
      DO 1 I=,NN
      IF (A(I).LT.A(I+1)) GO TO 1
      IORDER=IORDER+1
      TEMP=INDEX(I+1)
      B=A(I+1)
      INDEX(I+1)=INDEX(I)
      A(I+1)=A(I)
      INDEX(I)=TEMP
      A(I)=B
1     CONTINUE
      IF (IORDER.EQ.0) GO TO 3
2     CONTINUE
3     CONTINUE
      RETURN
      END
```

Appendix D

Extrapolation and Interpolation for Evaluating the Missing Reference Eigenvalues

A problem arose in calculating the rms deviation since Burdick did not list some of the nine lowest band energies in his paper (Ref. 8). These missing eigenvalues are mostly in the higher bands. To obtain these missing eigenvalues, extrapolation and interpolation from nearby eigenvalues were used. Because of the limitation of these methods, some extrapolated and interpolated eigenvalues may not be very reliable. We attempted to extrapolate and interpolate the missing eigenvalues carefully from as many directions in the Brillouin zone as possible for checking. After trials, it was decided that only missing values below the sixth band would be obtained in this fashion for the computation of the rms deviation. The actual extrapolations and interpolations are shown in Figs. D-1 – D-12. The missing eigenvalues which were obtained with these methods are those at points (332) for 5^{th} band, (281), (343), and (353) for the 6^{th} band.

As can be seen from Figs. D-1 – D-6, the extrapolated eigenvalues at (281) for the 6^{th} band and at (332) for the 5^{th} band are of -0.099 and -0.572 rydbergs respectively. The crosses in Figs. D-1 and D-2 are the reference eigenvalues at corresponding points which was taken into account as a help for the extraction.

From Figs. D-7 – D-10, the extrapolated eigenvalues at (343) for the 6^{th} band are -0.502 and -0.533 rydbergs and at (353) for the same band are -0.378 and -0.399 rydbergs respectively. It can be seen that the extrapolated values at these points are not comparable, having difference of more than 0.01 rydberg.

Figs. D-11 and D-12 show the interpolation of eigenvalues at (353) in another direction with the help of eigenvalue at (343). After careful examination, we finally decided on the eigenvalues of -0.502 and -0.403 rydbergs for (343) and (353) respectively.

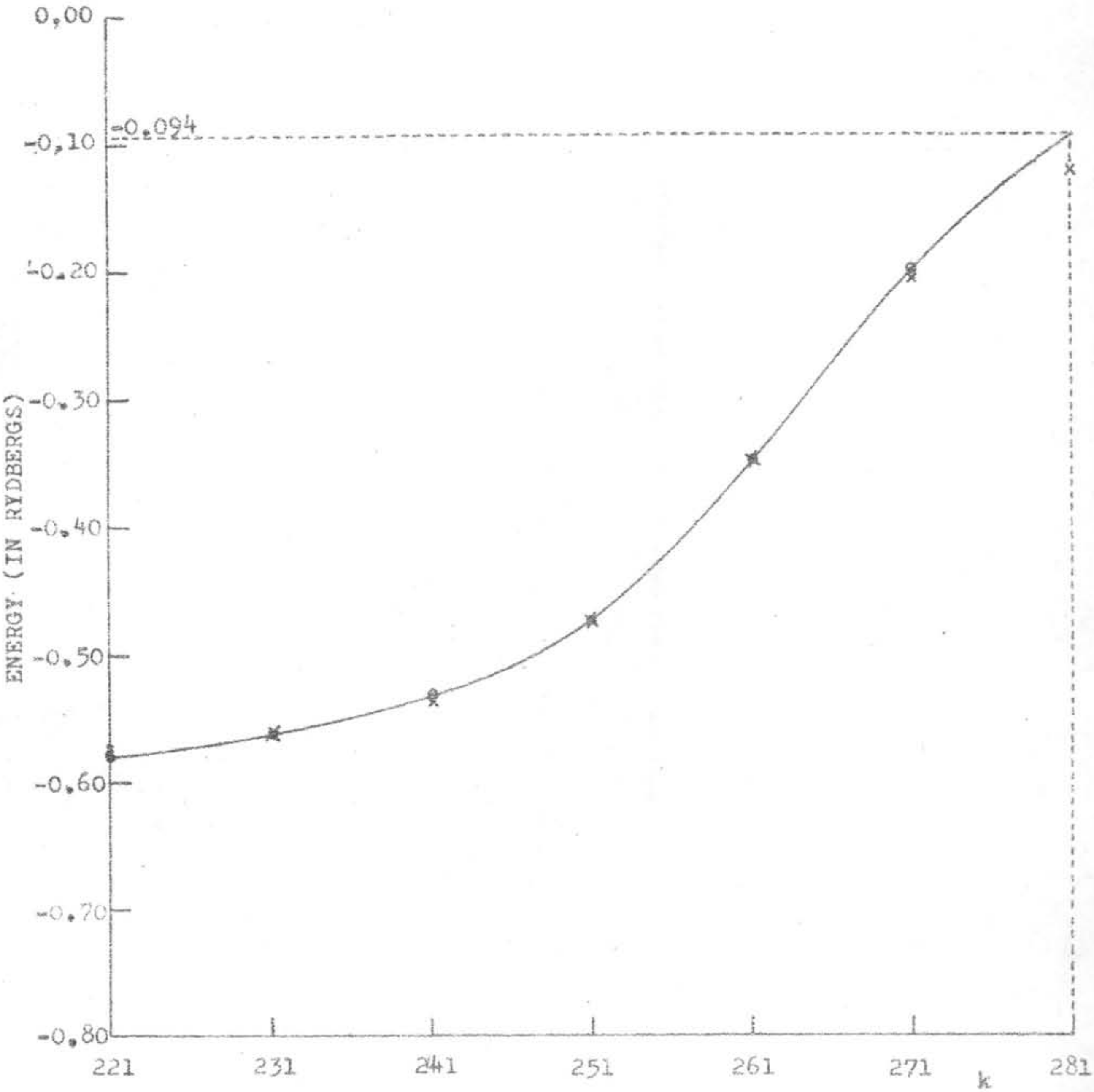
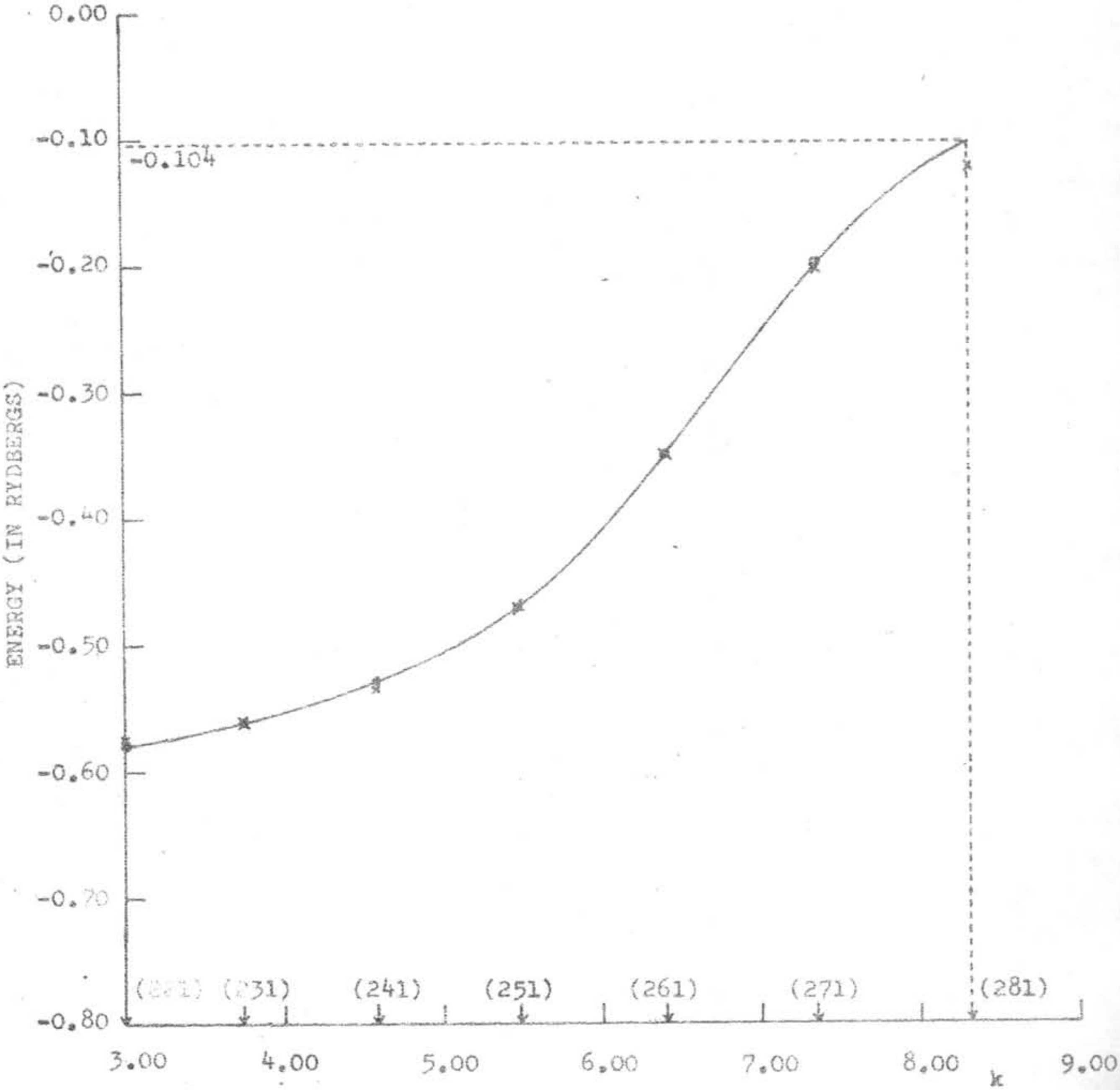

0,00
-0.094
-0,10
-0.20
-0.30
-0.40
-0.50
-0.60
-0.70
-0.80
ENERGY (IN RYDBERGS)
221
231
241
251
261
271
281
k

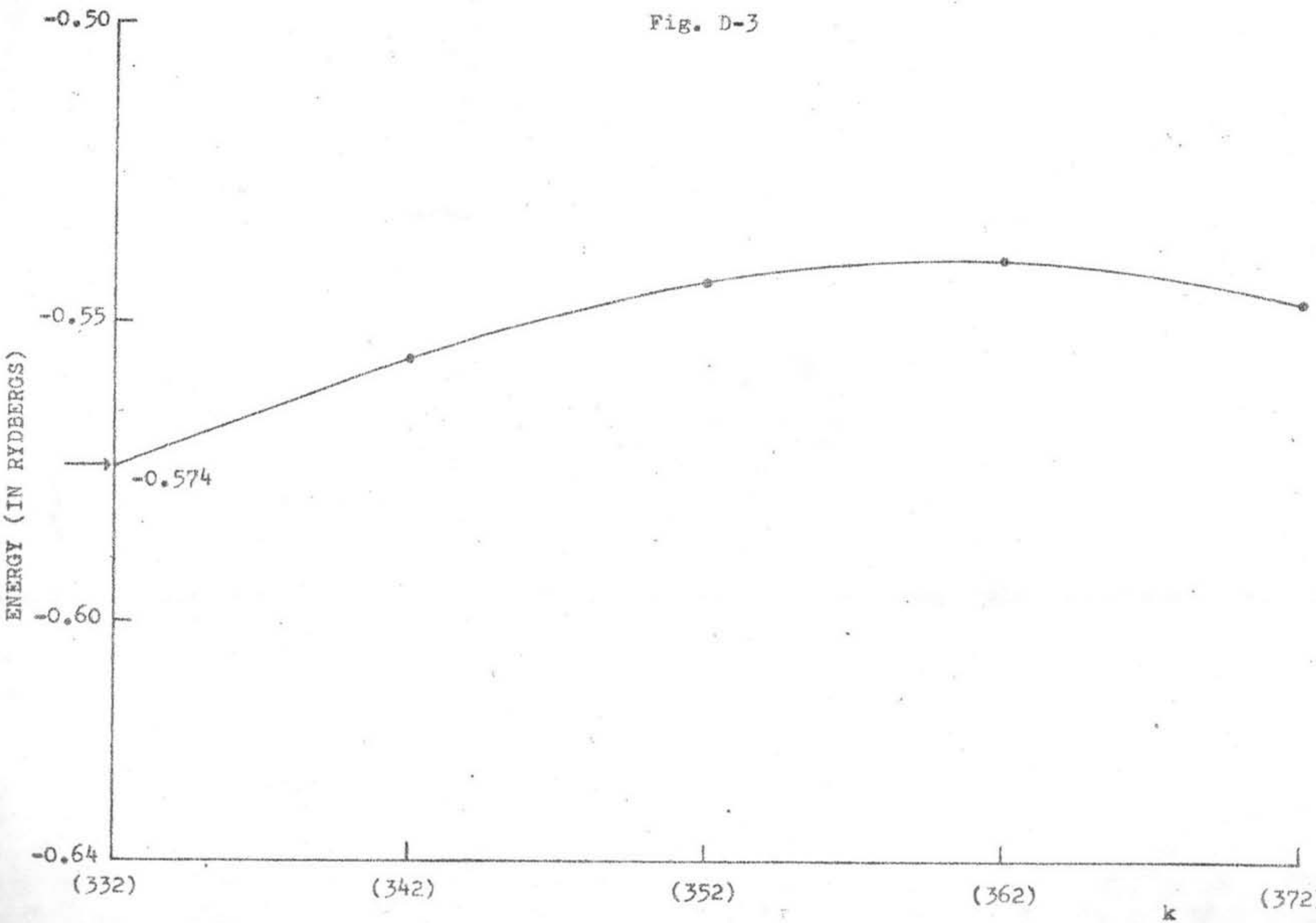
Fig. D-1



0.00
-0.10
-0.104
-0.20
-0.30
-0.40
-0.50
-0.60
-0.70
-0.80
ENERGY (IN RYDBERGS)
(231)
(241)
(251)
(261)
(271)
(281)
3.00
4.00
5.00
6.00
7.00
8.00
k
9.00

Fig. D-2

Fig. D-3



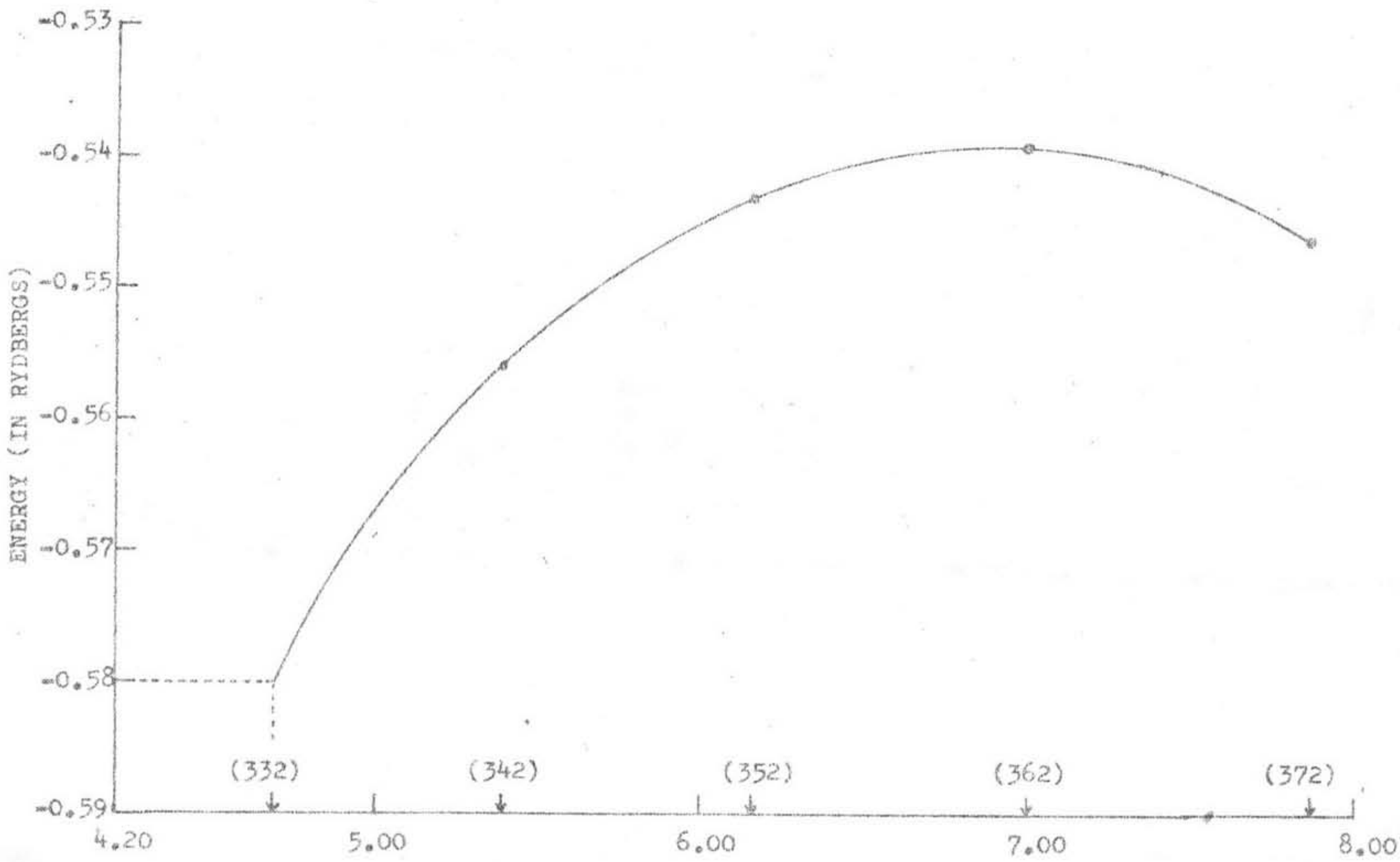

-0.53
-0.54
-0.55
-0.56
-0.57
-0.58
-0.59
ENERGY (IN RYDBERGS)
(332)
(342)
(352)
(362)
(372)
4.20
5.00
6.00
7.00
8.00
k

Fig. D-4

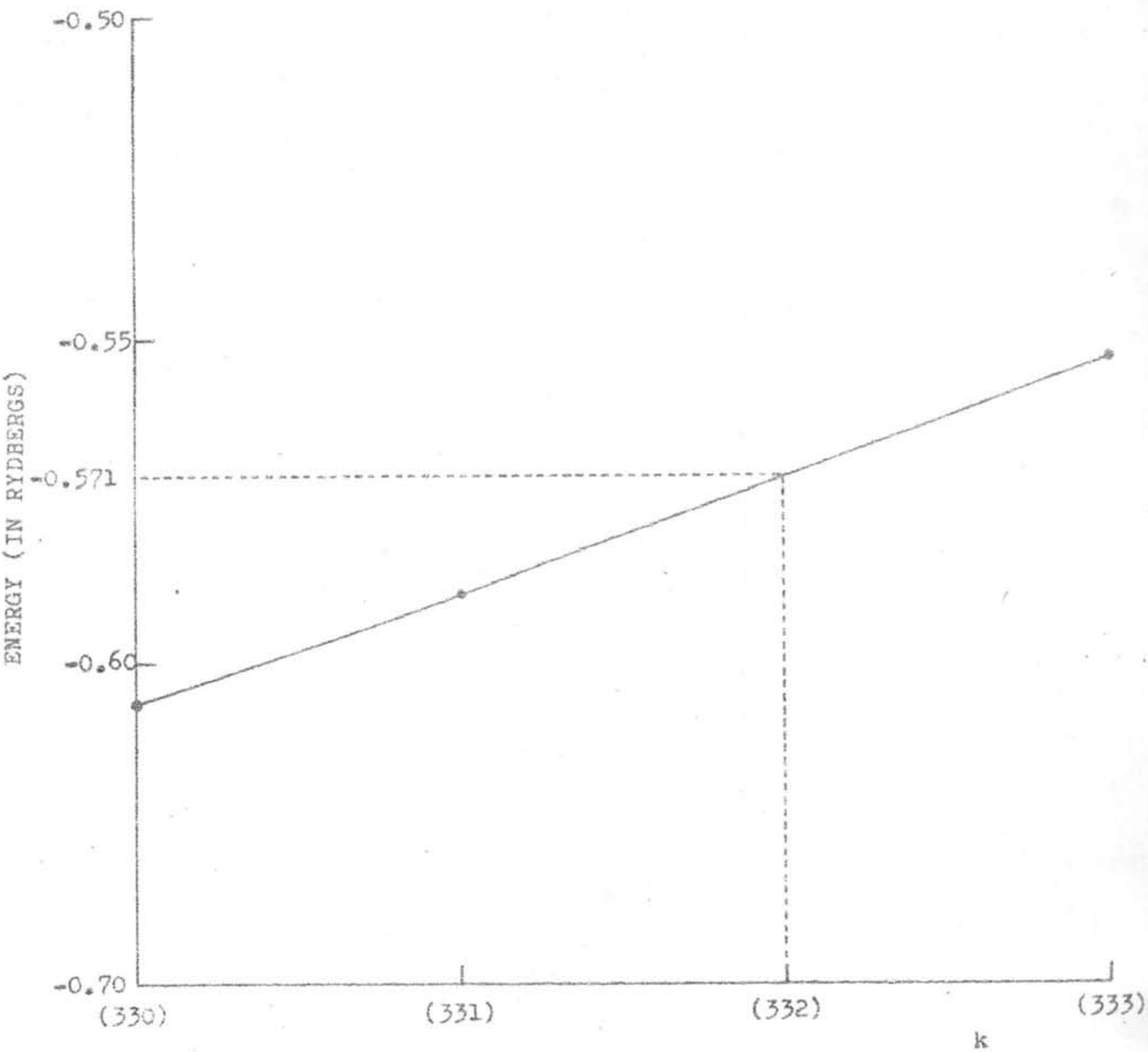
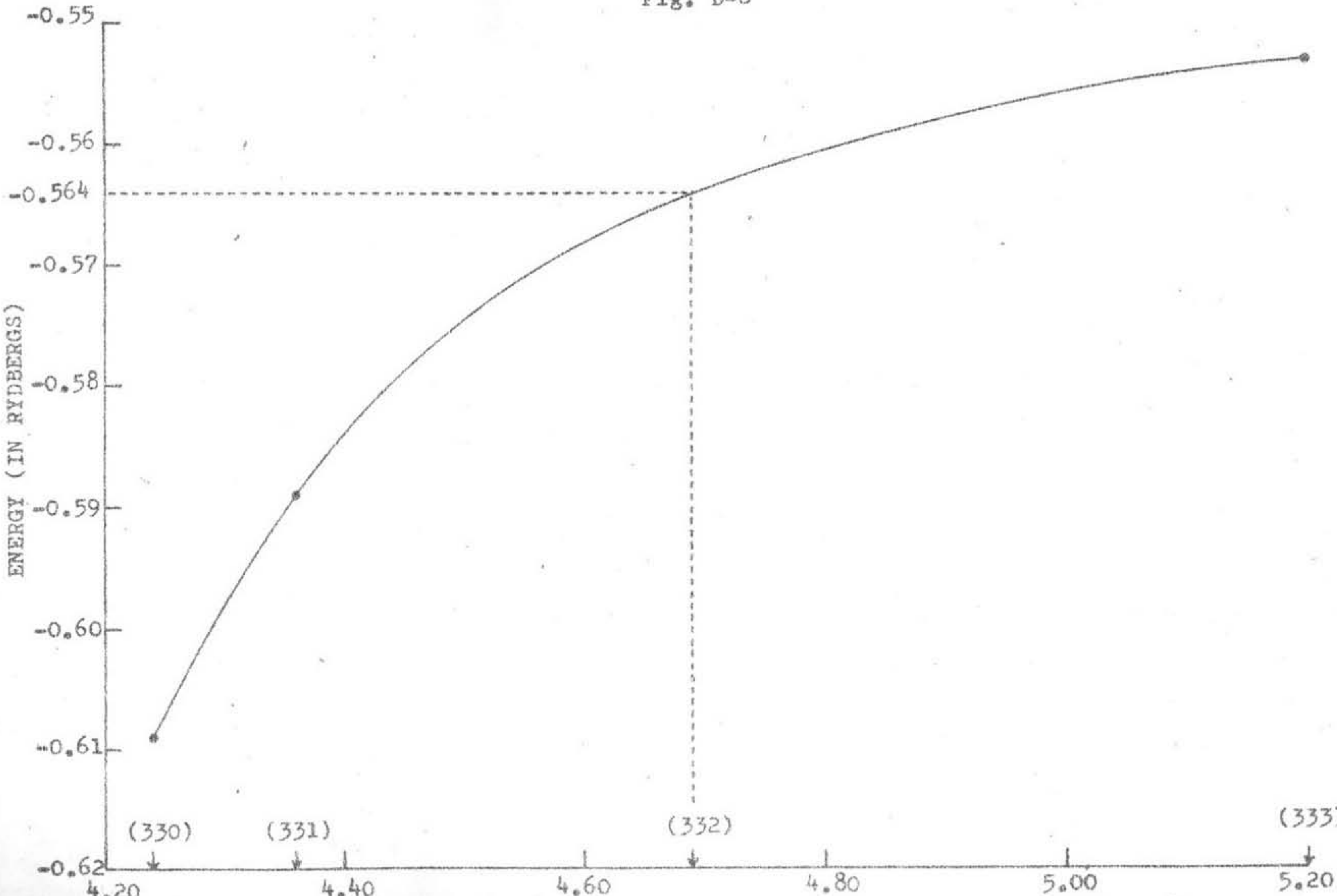


Fig. D-5

Fig. D-6



-0.55
-0.56
-0.564
-0.57
-0.58
-0.59
-0.60
-0.61
-0.62
ENERGY (IN RYDBERGS)
(330)
(331)
(332)
(333)
4.20
4.40
4.60
4.80
5.00
5.20
k

Fig. D-7

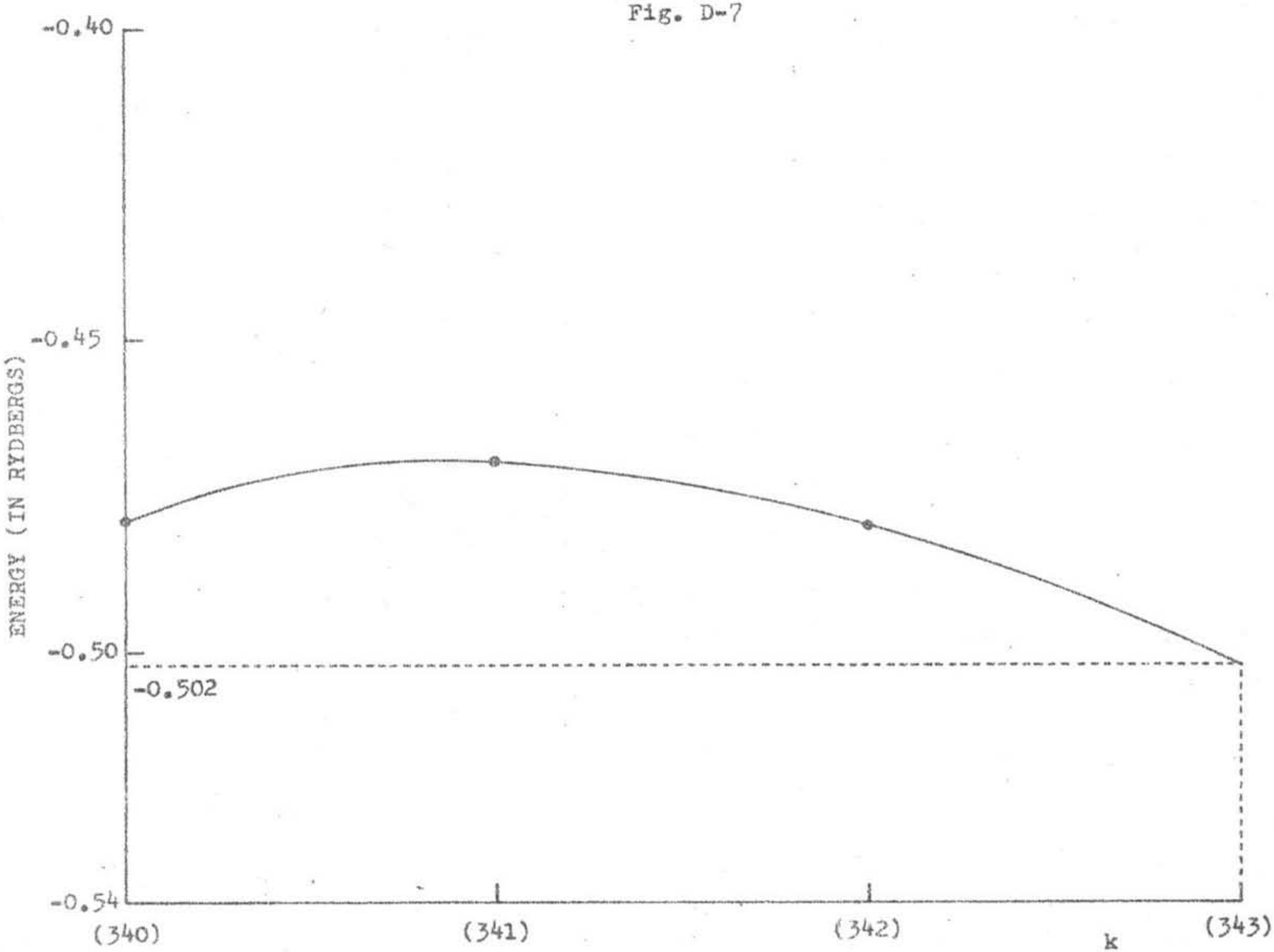
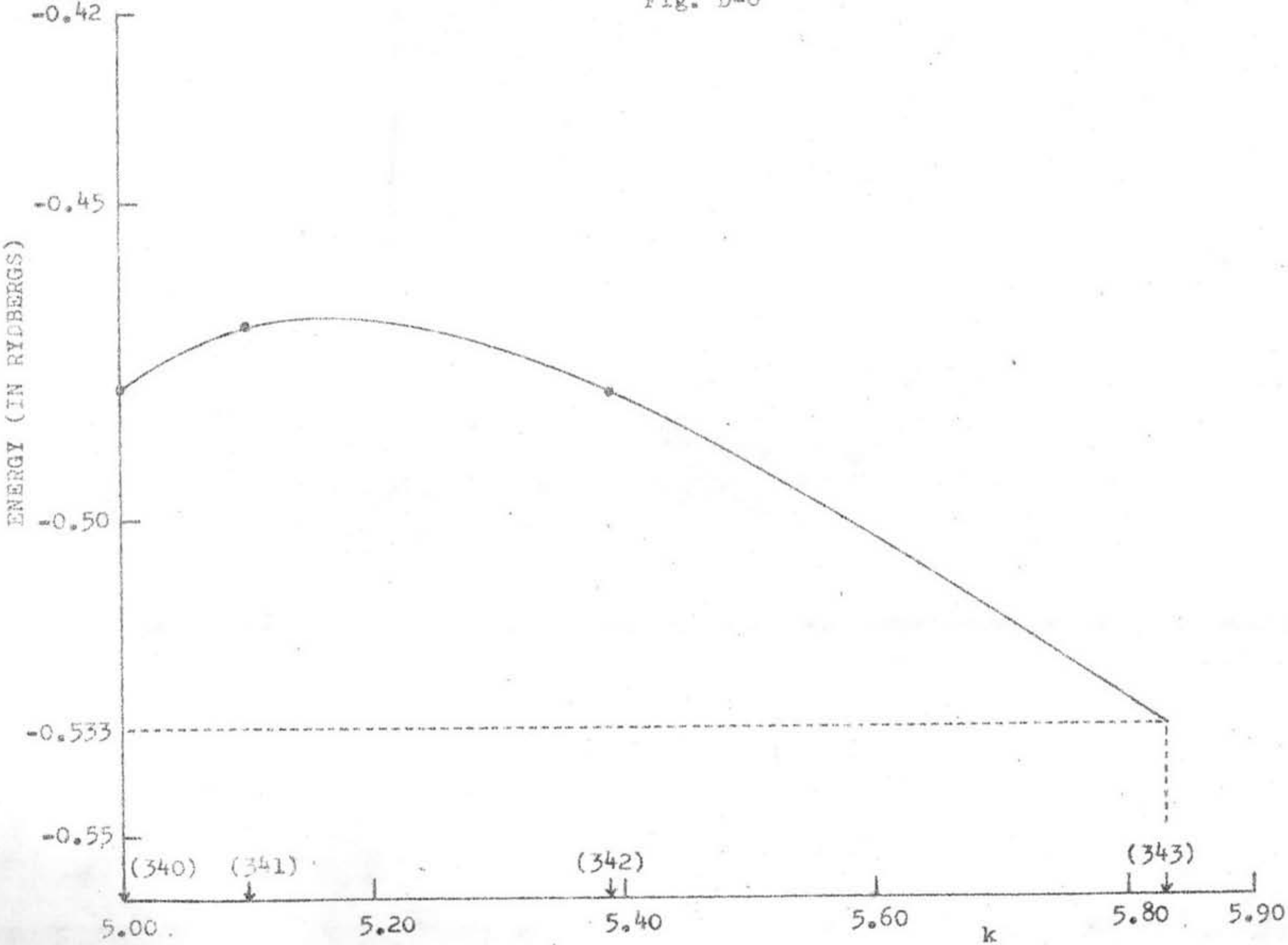


Fig. D-8



-0.42
-0.45
-0.50
-0.533
-0.55
ENERGY (IN RYDBERGS)
(340)
(341)
(342)
(343)
5.00
5.20
5.40
5.60
5.80
5.90
k

Fig. D-9

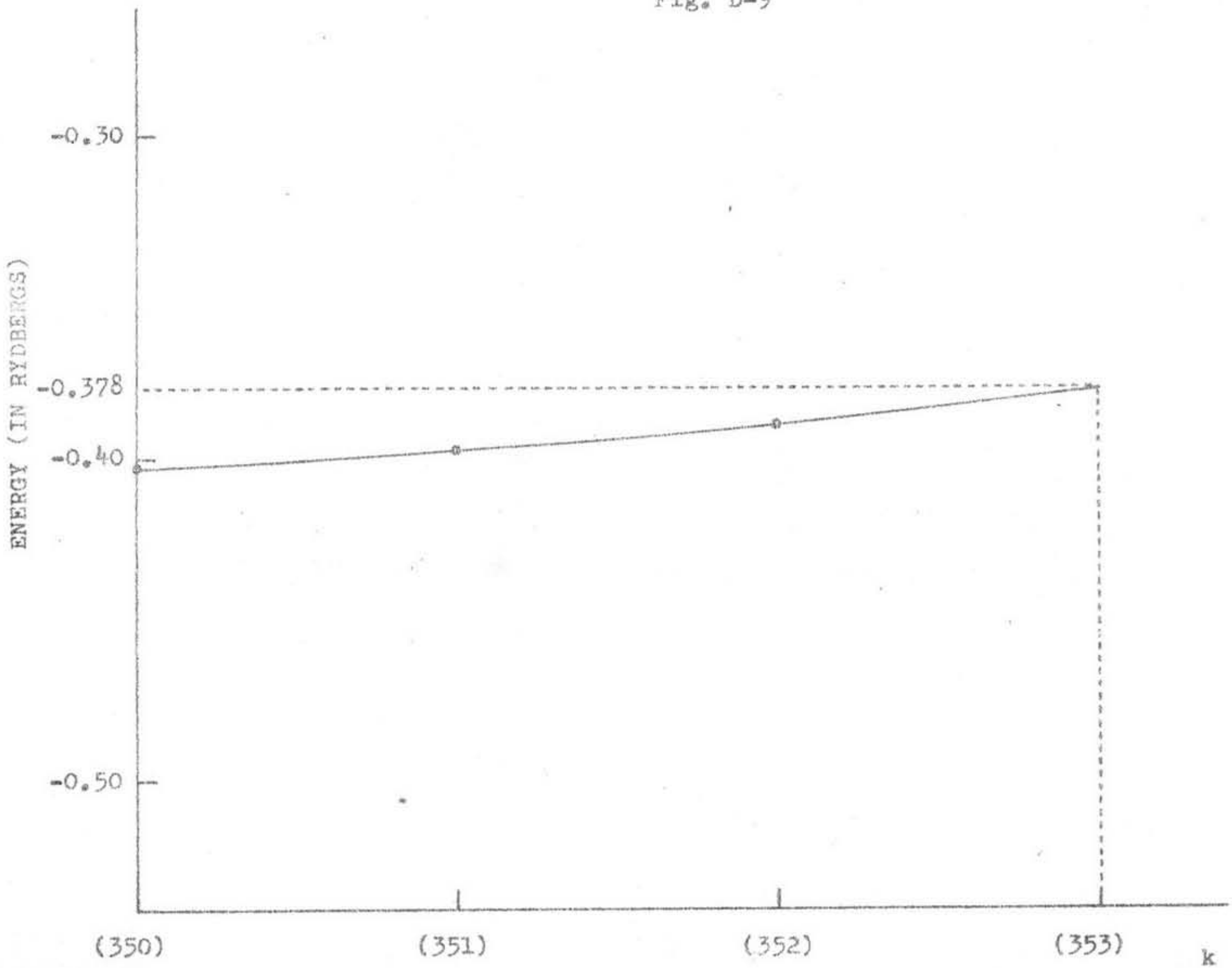
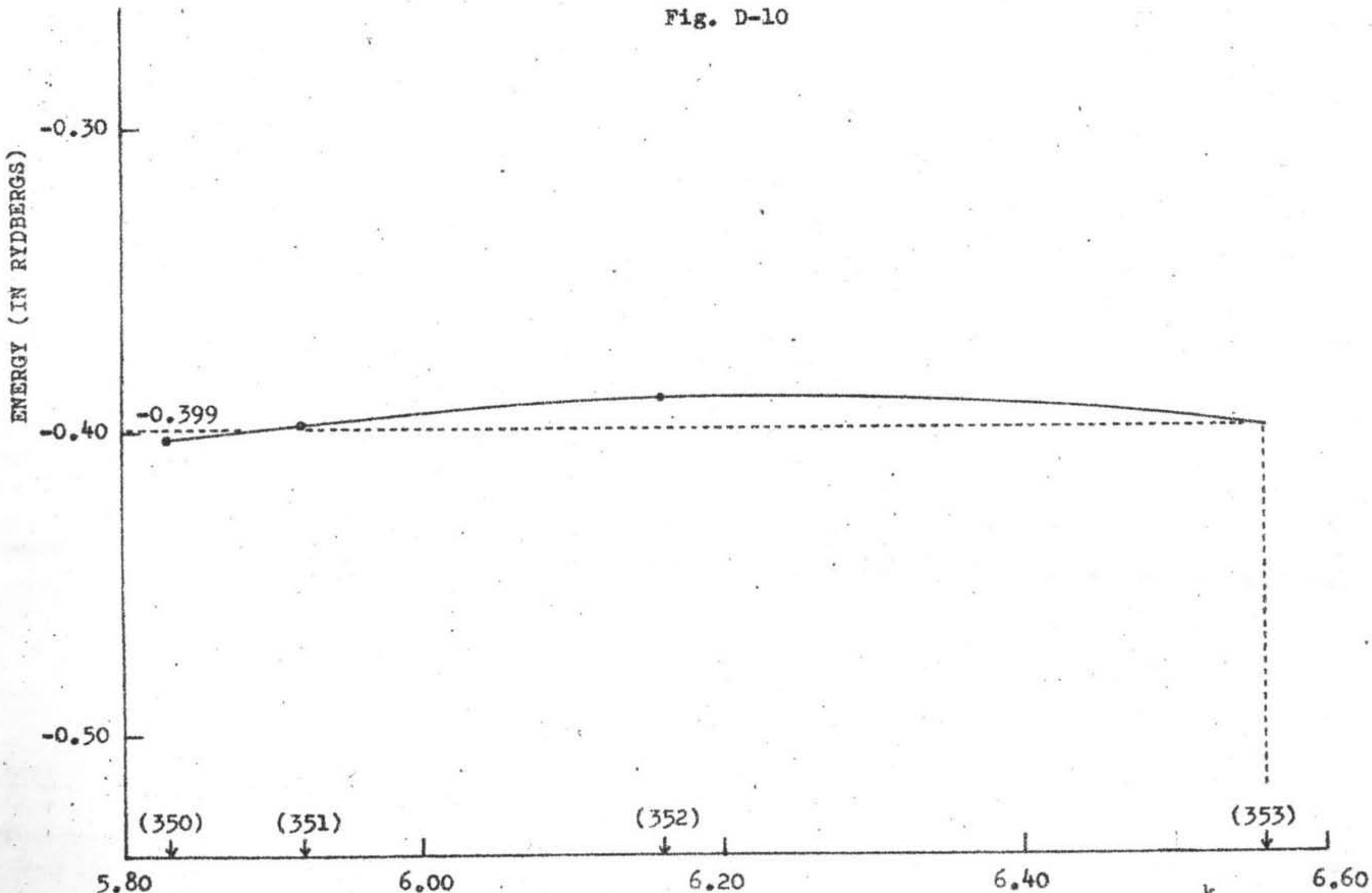


Fig. D-10



ENERGY (IN RYDBERGS)
-0.30
-0.399
-0.40
-0.50
(350)
(351)
(352)
(353)
5.80
6.00
6.20
6.40
6.60
k

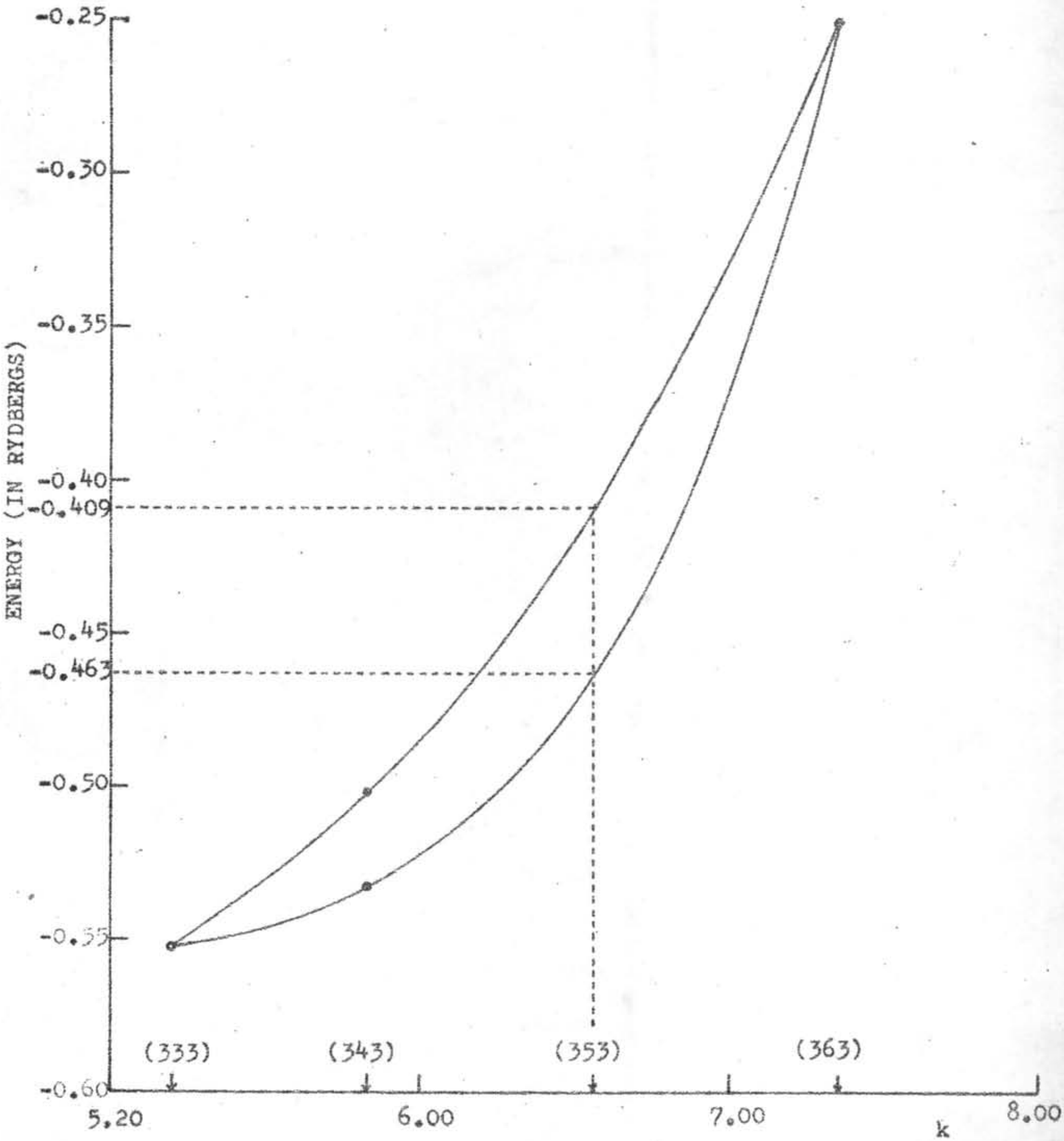

ENERGY (IN RYDBERGS)
-0.25
-0.30
-0.35
-0.40
-0.409
-0.45
-0.463
-0.50
-0.55
-0.60
(333)
(343)
(353)
(363)
5.20
6.00
7.00
8.00
k

Fig. D-11

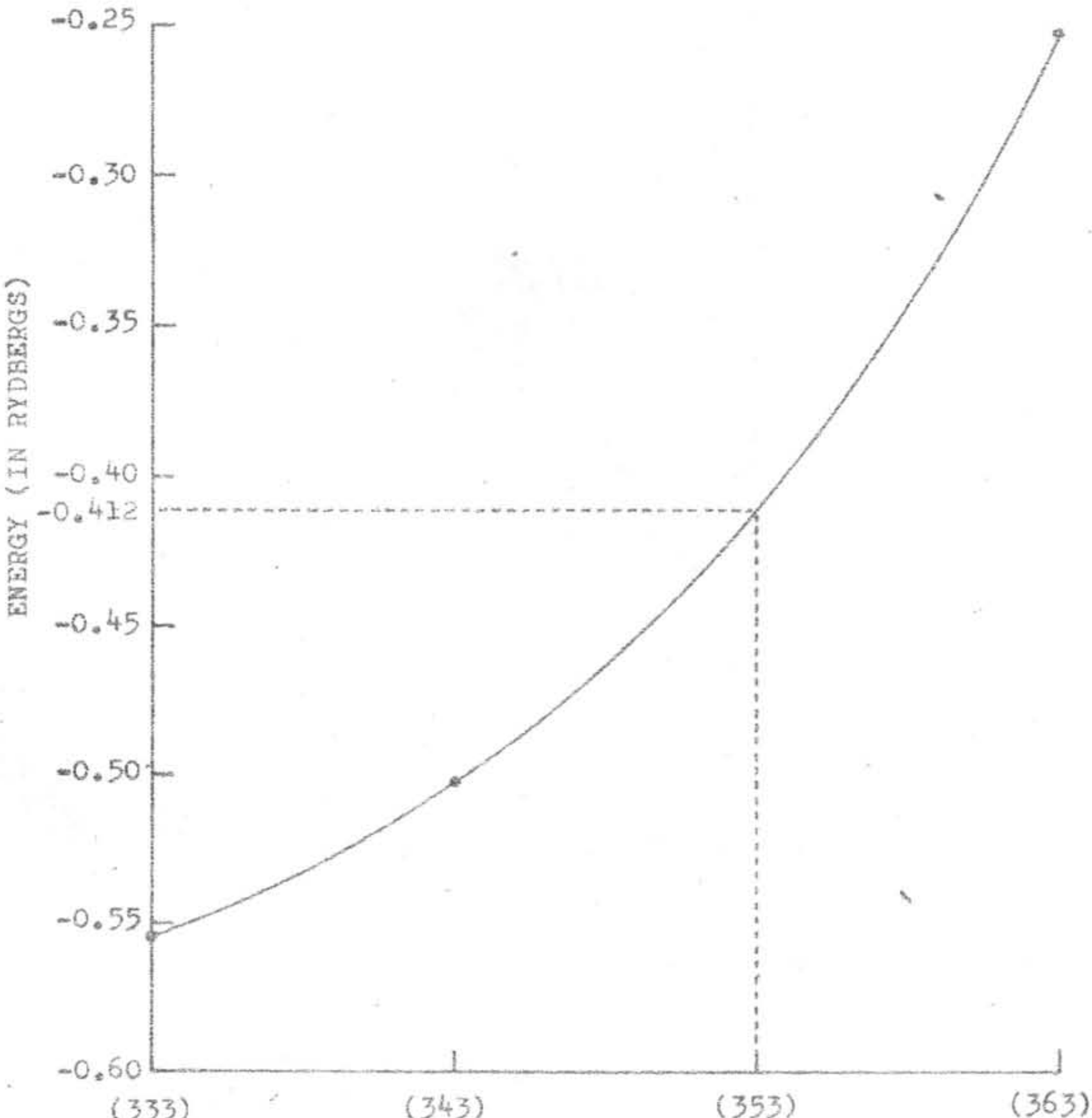

-0.25
-0.30
-0.35
ENERGY (IN RYDBERGS)
-0.40
-0.412
-0.45
-0.50
-0.55
-0.60
(333)
(343)
(353)
(363)
k

Fig. D-12