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APPENDIX A

INTEGRATION PROCEDURE SUGGESTED BY SOMMERFELD

a). The integral of the form

$$J_1 = \oint \sqrt{A + \frac{2B}{r} - \frac{C}{r^2}} dr \quad (A.1)$$

has two branch points, r_{\min} and r_{\max} , which have real positive values A , B , and C in eq.(A.1) are some constants.

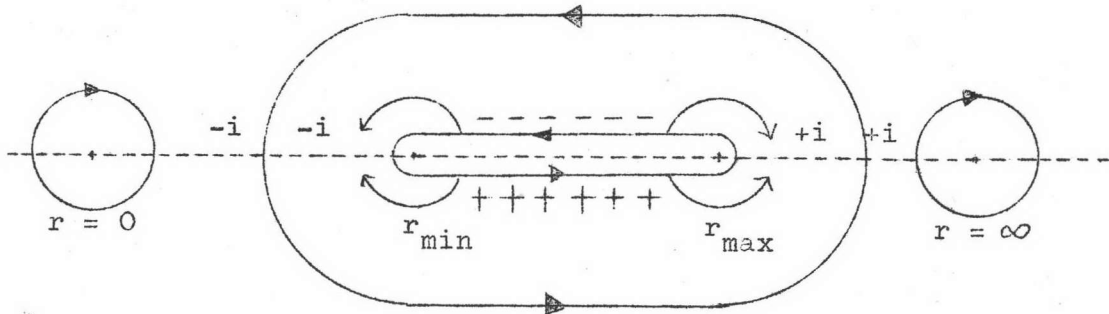


Fig. A.1

The r plane is supposed to be slit up between r_{\min} and r_{\max} and represent the upper sheet of a two-surface Riemann sheet. On account of the positive character of phase integral, the sign of the square root is taken to be positive for a positive dr (section below the slit) and negative for a negative dr (section above the slit). The square root on the real axis of the r plane outside the slit is imaginary and indeed positive and

imaginary for $r > r_{\max}$, negative and imaginary for $0 < r < r_{\min}$.

The poles of the integrand are at $r=0$ and $r=\infty$. Since the sign in front of the square root in the integrand must be negative for the region along the real axis below r_{\min} , the

integrand is represent as $-\sqrt{A + \frac{2B}{r} - \frac{C}{r^2}}$. The integrand is

expanded and it is found that the residue at the point $r=0$ is $-\sqrt{-C}$.

Since the square root on the real axis above r_{\max} is positive, the

integral becomes $-\int \sqrt{A + 2Bs - Cs^2} \frac{ds}{s^2}$ by setting $r = 1/s$.

By expanding the integrand we find the residue at $r = \infty$ is $-B/\sqrt{A}$.

By applying the Residue Theorem we obtain

$$J_1 = -2\pi i \left(-\sqrt{-C} - B/\sqrt{A} \right). \quad (A.2)$$

We see that J_1 will be real for $C > 0$ and $A < 0$. If we start

with the integrand $\sqrt{A + \frac{2B}{r} + \frac{C}{r^2}}$ we will obtain the total result

$$J_1 = -2\pi i \left(\sqrt{C} - B/\sqrt{A} \right) \quad (A.3)$$

which is real if $A < 0$ and $C < 0$.

b) The integral of the form

$$J_2 = \oint \sqrt{A + \frac{2B}{r} + \frac{C}{r^2} + \frac{D_1}{r^3} + \frac{D}{r^4}} dr \quad (A.4)$$

has the same two branch points as J_1 . Therefore we can still use the integration path given in Fig.A.1. D_1 and D in eq.(A.4) are constants.

Excluding all powers higher than D_1 , D_1^2 and D we get upon expanding the integrand

$$\sqrt{A + \frac{2B}{r} + \frac{C}{r^2} + \frac{D_1}{r^3} + \frac{D}{r^4}} = \sqrt{A + \frac{2B}{r} + \frac{C}{r^2}} + \frac{1}{2} \left(A + \frac{2B}{r} + \frac{C}{r^2} \right)^{-1/2} \left(\frac{D_1}{r^3} + \frac{D}{r^4} \right) - \frac{1}{8} \left(A + \frac{2B}{r} + \frac{C}{r^2} \right)^{-3/2} \frac{D_1^2}{r^6} \dots$$

The integral becomes

$$J_2 = J_1 + \frac{D_1}{2} J_3 + \frac{D}{2} J_4 - \frac{D_1^2}{8} J_5 \quad (\text{A.5})$$

where $J_3 = \oint \left(A + \frac{2B}{r} + \frac{C}{r^2} \right)^{-1/2} \frac{dr}{r^3}$, (A.6)

$$J_4 = \oint \left(A + \frac{2B}{r} + \frac{C}{r^2} \right)^{-1/2} \frac{dr}{r^4}, \quad (\text{A.7})$$

and $J_5 = \oint \left(A + \frac{2B}{r} + \frac{C}{r^2} \right)^{-1/2} \frac{dr}{r^6}$. (A.8)

These integrals can be performed by the same procedure as that applied to J_1 . The results are

$$J_3 = 2\pi i \frac{B}{\sqrt{C}}, \quad (\text{A.9})$$

$$J_4 = \frac{\pi i}{\sqrt{C}} \left(\frac{A}{C} - \frac{3B^2}{C^2} \right), \quad (\text{A.10})$$

and $J_5 = \frac{3\pi i}{C\sqrt{C}} \left(\frac{A}{C} - \frac{5B^2}{C^2} \right)$. (A.11)

Eq.(A.5) now becomes

$$J_2 = -2\pi i \left\{ \sqrt{C} - \frac{B}{\sqrt{A}} - \frac{1}{2c\sqrt{C}} \left(D_1 - \frac{3}{2} \frac{DB}{C} + \frac{15}{8} \frac{D_1^2 B}{C^2} \right) - \frac{1}{4c\sqrt{C}} \left(D - \frac{3}{4} \frac{D_1^2}{C} \right) \right\} \quad (A.12)$$

For $D_1 = 0$, we have

$$J_2 = -2\pi i \left\{ \sqrt{C} - \frac{B}{\sqrt{A}} + \frac{3}{4} \frac{DB^2}{c^2\sqrt{C}} - \frac{1}{4} \frac{AD}{c\sqrt{C}} \right\} \quad (A.13)$$

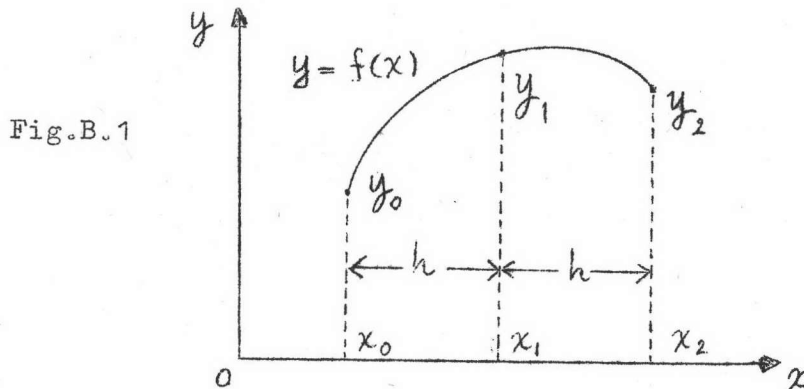
If A and C themselves are negative, we can rewritten eq.(A.13) to be

$$J_2 = 2\pi \left\{ \frac{B}{\sqrt{-A}} - \sqrt{-C} + \frac{D}{4c\sqrt{-C}} \left(\frac{3}{c} B^2 - A \right) \right\} \quad (A.14)$$

APPENDIX B

SIMPSON'S INTEGRATION FORMULA

The following Simpson's integration formula is adapted from Demidovich and Maron (1976).



The three-point integration as shown above is found to be

$$\int_{x_0}^{x_2} f(x) dx = \frac{h}{3}(y_0 + 4y_1 + y_2) \quad (\text{B.1})$$

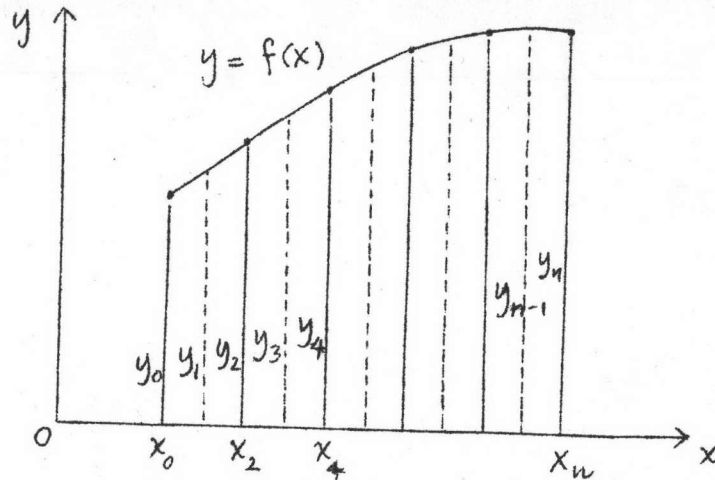
and the remainder

$$R = -\frac{h^5}{90} f^{(iv)}(\xi), \quad x_0 < \xi < x_2 \quad (\text{B.2})$$

The proper integration result will be obtained if the interval h tends to zero. We will divide the integration limits to be n intervals as shown. n must be an even integer because we want to apply the integration formula obtained in eq.(B.1) on each interval pair. We have

$$\int_{x_0}^{x_n} f(x) dx = \frac{h}{3}(y_0 + 4y_1 + y_2) + \frac{h}{3}(y_2 + 4y_3 + y_4) + \dots + \frac{h}{3}(y_{2n-2} + 4y_{2n-1} + y_n)$$

Fig.B.2



$$\int_{x_0}^{x_n} f(x) dx = \frac{h}{3} \left[y_0 + y_n + 4(y_1 + y_3 + \dots + y_{n-1}) + 2(y_2 + y_4 + \dots + y_{n-2}) \right] \quad (B.3)$$

Since we are concerned with an integral of the form

$$\int_{\rho_i}^{\rho_j} \left[\frac{\sqrt{(\alpha - \epsilon n / 2) \rho^2 + \beta \rho + (\gamma - \frac{1}{2}(\epsilon + \frac{1}{2})^2) - \delta / \rho^2}}{\rho} \right] d\rho ,$$

a program for this calculation is made. The program is shown in table B.1 and is appropriate to a calculator model HP-97. The user instructions are given in table B.2 .

The program can be adapted to the integration from ρ_{min} to ρ_j . In this case , the value of $\Delta \rho$ is negative, thus some steps in the program must be changed. The steps 014 and 015 must be interchanged and an ABS key must be inserted between steps 044 and 045. The value of h must be set to be negative and thus we can use ρ_{min} instead of ρ_{max} . We are now able to calculate the integration by using the user instructions in table B.2 .

001	*LEL4	21 11	036	*LBL2	21 02	071	2	02
002	RCL5	36 02	037	RCL9	36 02	072	=	-24
003	3	03	038	ST-3	35-45 03	073	-	-45
004	=	-24	039	GSBe	23 16 15	074	ST0A	35 11
005	ST0E	35 12	040	SFC	16-11	075	RCL2	36 02
006	GSBe	23 16 15	041	PRTX	-14	076	.	-62
007	SFC	16-11	042	RCL5	36 15	077	5	05
008	PRTX	-14	043	ST-4	35-45 04	078	+	-55
009	x	-35	044	RCL4	36 04	079	X ²	53
010	ST04	35 04	045	SFC	16-11	080	2	02
011	*LBL1	21 01	046	PRTX	-14	081	=	-24
012	RCL9	36 02	047	R/S	51	082	CHS	-22
013	ST+3	35-55 03	048	*LBLe	21 16 15	083	RCL8	36 02
014	RCL5	36 03	049	RCL4	36 11	084	+	-55
015	RCL3	36 03	050	RCL3	36 03	085	STDC	35 17
016	XYY?	16-24	051	X ²	53	086	RTN	24
017	GT02	22 02	052	x	-35	087	*LBLB	21 12
018	CLX	-51	053	RCL7	36 07	088	RCL4	36 04
019	GSBe	23 16 15	054	RCL3	36 03	089	SFC	16-11
020	RCL6	36 12	055	x	-35	090	PRTX	-14
021	x	-35	056	+	-55	091	RTN	24
022	ST0E	35 15	057	RCLC	36 13	092	*LBLe	21 14
023	4	04	058	+	-55	093	RCL1	36 46
024	x	-35	059	RCLD	36 14	094	ST+3	35-55 03
025	ST+4	35-55 04	060	RCL3	36 03	095	GSBe	23 16 15
026	RCL9	36 03	061	X ²	53	096	GT0D	22 14
027	ST+3	35-55 03	062	=	-24	097	RTN	24
028	GSBe	23 16 15	063	+	-55	098	*LBLe	21 15
029	RCLB	36 12	064	JX	54	099	RCL1	36 46
030	x	-35	065	RCL3	36 03	100	ST-3	35-45 03
031	ST0E	35 15	066	=	-24	101	RCL3	36 03
032	2	02	067	RTN	24	102	ST05	35 05
033	x	-35	068	*LBLa	21 16 11	103	R/S	51
034	ST+4	35-55 04	069	RCL6	36 06			
035	GT01	22 01	070	RCL0	36 00			

Registers

0	E_{nl}	1	-	2	l	3	P_i
4	Int.result	5	P_j	6	d	7	β
8	γ	9	h	A	$A = d - E_{nl}/2$	B	$h/3$
C	$C = \gamma - \frac{1}{2}(l + \frac{1}{2})^2$	D	δ	E	cal.memory	I	Δp

Table B.1 Integration Program

STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS	OUTPUT DATA/UNITS
1	Load side 1 of program			
2	Load input data	E_{nl}	STO 0	E_{nl}
		l	STO 2	l
		ρ_i	STO 3	ρ_i
		ρ_j	STO 5	ρ_j
		α	STO 6	α
		β	STO 7	β
		γ	STO 8	γ
		h	STO 9	h
		δ	STO D	δ
3	Start the calculation		f a	C
4	If ρ_j is not a ρ_{max} and is known, go to step 8			
5	Solve for ρ_{max}			
	5.1 find possible $\rho_j < \rho_{max}$	$\Delta \rho_j$	STO I	$\Delta \rho_j$
	(now ρ is greater than ρ_{max})		D	error
	5.2 set ρ_j to be $\rho_j - \Delta \rho_j$ automatically		CLX	
			E	
6	Adjust ρ_j by setting a new suitable $\Delta \rho_j$ as fine as you need and repeat step 5 again			
7	Set ρ_i and h	ρ_i	STO 3	ρ_i
		h	STO 9	h
8	Integration		A	$f(\rho_i)$
				$f(\rho_j)$
				Int.result

Table B.2 User instructions

for Simpson's integration formula

APPENDIX C

DETERMINATION OF PARAMETERS

The parameters are determined from the quantization condition and the matching conditions by solving the following equations simultaneously.

$$n-l-\frac{1}{2} = \frac{\sqrt{2}}{\pi} \left[\left\{ F_2 - G_2(\beta_j) \right\} + \left\{ G_1(\beta_j) - G_1(\beta_i) \right\} + \left\{ G_0(\beta_i) + F_0 \right\} \right], \quad (C.1)$$

$$\beta_{m+1} = 2(\alpha_m - \alpha_{m+1})\beta_i + \beta_m, \quad (C.2)$$

$$\gamma_{m+1} = (\alpha_{m+1} - \alpha_m)\beta_i^2 + \gamma_m. \quad (C.3)$$

All terms in the above equations have been defined in chapter IV. It is noted that if there exists two integrals in the quantization expression, the terms in the middle curly brackets in eq.(C.1) will disappear and the index "2" changes to "1" automatically.

The program designed for the case without polarization is given in table C.1 and the user instructions are given in table C.2 and C.3.

001	*LBLA	21 11	035	ST07	35 07	069	x	-35	103	x	-35
002	RCL6	36 06	036	2	02	070	2	02	104	Fi	16-24
003	RCL8	36 08	037	+	-24	071	RCL6	36 15	105	+	-24
004	2	02	038	RCLA	36 11	072	+	-35	106	RTN	24
005	+	-24	039	CHS	-22	073	+	-55	107	0	00
006	-	-45	040	JX	54	074	RCL3	36 03	108	STOD	35 14
007	ST0A	35 11	041	+	-24	075	+	-24	109	RCL9	36 09
008	RCL3	36 03	042	ST0B	35 12	076	GSBa	23 16 11	110	ST+6	35-55 06
009	AF	53	043	RCL6	36 15	077	+	-24	111	GT0A	22 11
010	RCL6	36 06	044	CHS	-22	078	RAD	16-22	112	*LBLa	21 16 11
011	RCL4	36 04	045	JX	54	079	SIN ⁻¹	16 41	113	RCL7	36 07
012	-	45	046	-	-45	080	RCL6	36 15	114	X ²	53
013	x	-35	047	Fi	16-24	081	CHS	-22	115	4	04
014	RCL1	36 01	048	x	-35	082	JX	54	116	RCLA	36 11
015	+	-35	049	2	02	083	x	-35	117	x	-35
016	ST0B	35 06	050	+	-24	084	RCL1	36 46	118	RCL6	36 15
017	RCL2	36 02	051	RTN	24	085	+	-55	119	x	-35
018	.	-02	052	*LBLA	21 11	086	RTN	24	120	-	-45
019	5	05	053	2	02	087	*LBLE	21 15	121	JX	54
020	+	-55	054	RCLA	36 11	088	RCLC	36 13	122	RTN	24
021	X ²	53	055	x	-35	089	+	-55	123	*LBLk	21 16 12
022	2	02	056	RCL3	36 03	090	STOD	35 13	124	RCL3	36 03
023	+	-24	057	x	-35	091	RTN	24	125	X ²	53
024	-	-45	058	RCL7	36 07	092	*LBLD	21 14	126	RCLA	36 11
025	ST0E	35 15	059	+	-55	093	RCLD	36 14	127	x	-35
026	RCL4	36 04	060	GSBa	23 16 11	094	+	-55	128	RCL3	36 03
027	RCL6	36 06	061	+	-24	095	STOD	35 14	129	RCL7	36 07
028	-	-45	062	RAD	16-22	096	RTN	24	130	x	-35
029	2	02	063	SIN ⁻¹	16 41	097	*LBLB	21 15	131	+	-55
030	x	-35	064	RCLB	36 12	098	RCLD	36 14	132	RCL6	36 15
031	RCL3	36 03	065	x	-35	099	RCLC	36 13	133	+	-55
032	x	-35	066	ST0I	35 46	100	+	-55	134	JX	54
033	RCL5	36 05	067	RCL7	36 07	101	2	02	135	RTN	24
034	+	-55	068	RCL3	36 03	102	JX	54	136	R/S	51

Registers

0	ϵ_{nl}	1	γ_0	2	l	3	β_i
44	α_0	5	β_0	6	α_1	7	β_1
8	γ_1	9	$\Delta \alpha_1$	A	A	B	$B/2\sqrt{A}$
C	SUM C	D	SUM D	E	C	I	

Table C.1 Parameter determination program

STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS	OUTPUT DATA/UNITS
	<p>This program may be employed to calculate f_{min} of $Q(\rho)$ of any state</p> <p>1 Load side 1 and side 2 of program</p> <p>2 Calculate f_{min} of an f state</p> <p>2.1 Load input data</p> <p>2.2 Start the calculation</p> <p>2.3 Calculate f_{min}</p>	E_{nl} $\alpha_0 = 0$ $\beta_0 = 1$ $\gamma_0 = 0$ $l = 3$ $\alpha_1 = 0$	STO 0 STO 4 STO 5 STO 1 STO 2 STO 6 A f RCL 7 - 2 ÷ RCL A ÷	E_{nl} α_0 β_0 γ_0 l α_1 d Δ f_{min}
3	<p>Calculate f_{min} of a d state</p> <p>3.1 Reset E_{nl}, l and α_1 (known) by repeating some steps in 2.1</p> <p>3.2 Since $Q_0(\rho)$ have been determined, we can set f_i</p> <p>3.3 Repeat step 2.2 and 2.3</p>	f_i	STO 3	f_i
4	<p>Calculate f_{min} of a p state :</p> <p>The procedure is the same as that of a d state except α_0, β_0, and γ_0 must be changed to α_1, β_1, and γ_1, respectively</p>			

Table C.2 Instructions for calculating f_{min}

STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS	OUTPUT DATA/UNITS
	Determination of parameters			
1	Load side 1 and side 2 of program			
2	Calculate $F_0 + G_0(\rho_i)$ for any state			
	2.1 Load input data by repeating step 2.1 in table C.2			
	2.2 Load a selected ρ_i	ρ_i	STO 3	ρ_i
	2.3 Operate and store the functions in register C		A C B C	F_0 G_0
3	If there exists only two integrals, go to step 5.2 and use the index "1" instead of "2".			
4	Calculate $G_1(\rho_i)$ and $G_1(\rho_j)$			
	4.1 Set a new (known) α_1	α_1	STO 6	α_1
	4.2 Calculate $G_1(\rho_i)$ and deduct the register C		A B CHS C	$G_1(\rho_i)$ $-G_1(\rho_i)$
	4.3 Calculate $G_1(\rho_j)$ and sum within the register C	ρ_j	STO 3 B C	$G_1(\rho_j)$
5	Calculate $F_2 - G_2(\rho_j)$ and determine α_2			
	5.1 Replace zero-index parameters by 1-index parameters		RCL 6 STO 4 RCL 7 STO 5 RCL 3 STO 1	α_1 α_1 ρ_1 ρ_1 γ_1 γ_1

(Continued)

STEP	INSTRUCTIONS	INPUT DATA / UNITS	KEYS	OUTPUT DATA / UNITS
	5.2 Assume a value of α_2	α_2	STO 4	α_2
	5.3 Calculate F_2 and store in register D		A D	F_2
	5.4 Calculate $G_2(\rho_j)$ and deduct the register D		B CHS D	$-G_2(\rho_j)$
6	Testing			
	6.1 Calculate the right hand side of eq.(C.1)		E	RHS
	6.2 If $RHS > n - \frac{l-1}{2}$, set $\Delta\alpha_2 > 0$	$\Delta\alpha_2$	STO 9	$\Delta\alpha_2$
	6.3 Repeat step 5 (register D is clear automatically)		R/S	
7	Step 6 is repeated again and again till the right hand side is equal to $n - \frac{l-1}{2}$ as near as you need.			
8	After getting a satisfaction we recall the results from the registers		RCL 6 RCL 7 RCL 8	α_2 β_2 γ_2

Table C.3 Instructions for determining parameters

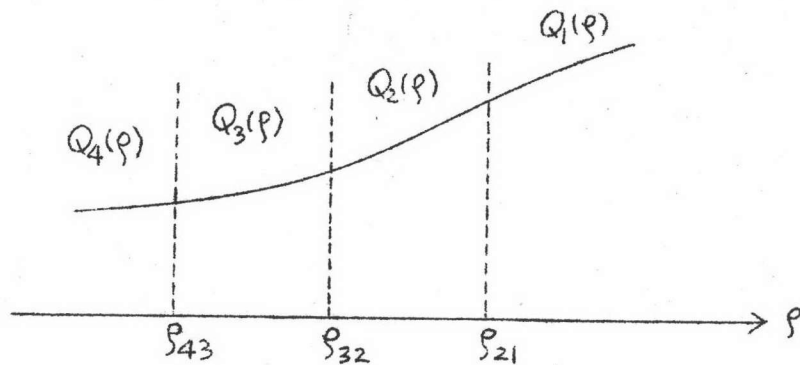
APPENDIX D

DETERMINATION OF MATCHING FUNCTIONS

If the functions $Q_3(\rho)$ and $Q_2(\rho)$ are created to match the function $Q_4(\rho)$ with the function $Q_1(\rho)$ at ρ_{43} , ρ_{32} and ρ_{21} respectively, we must solve six matching conditions simultaneously.

These equations are given in eq.(C.1) and eq.(C.2) where the running number n now runs from 1 to 3.

Fig.C.1



The program and the user instructions are given in table D.1 and table D.2 respectively. It is noted that the program can be employed to match any parabolic functions with the same matching conditions.

001	*LRLA	21 11	038	-	-45	075	+	-55	112	RCL3	36 03
002	RCL7	36 07	039	RCL7	36 07	076	PRTX	-14	113	RCL8	36 08
003	RCL8	36 08	040	X ²	53	077	RCL8	36 08	114	x	-35
004	-	-45	041	RCL6	36 06	078	X ²	53	115	-	-45
005	RCL7	36 07	042	X ²	53	079	RCLB	36 12	116	RCL8	36 08
006	X ²	53	043	-	-45	080	x	-35	117	X ²	53
007	RCL6	36 06	044	x	-35	081	RCL5	36 05	118	RCL7	36 07
008	X ²	53	045	RCL2	36 02	082	+	-55	119	X ²	53
009	-	-45	046	RCL5	36 05	083	PRTX	-14	120	-	-45
010	x	-35	047	-	-45	084	RCL2	36 02	121	x	-35
011	RCL6	36 06	048	RCL3	36 03	085	RCL5	36 05	122	-	-45
012	RCL7	36 07	049	RCL8	36 08	086	-	-45	123	RCLA	36 11
013	-	-45	050	X ²	53	087	RCL3	36 03	124	x	-35
014	RCL8	36 08	051	x	-35	088	RCL8	36 08	125	PRTX	-14
015	X ²	53	052	+	-55	089	X ²	53	126	CHS	-22
016	RCL7	36 07	053	RCL0	36 00	090	x	-35	127	RCL0	36 00
017	X ²	53	054	RCL6	36 06	091	+	-55	128	+	-55
018	-	-45	055	X ²	53	092	RCL0	36 00	129	RCL6	36 06
019	x	-35	056	x	-35	093	RCL6	36 06	130	x	-35
020	-	-45	057	-	-45	094	X ²	53	131	STOC	35 13
021	1/X	52	058	RCL6	36 06	095	x	-35	132	2	02
022	STOA	35 11	059	RCL7	36 07	096	-	-45	133	x	-35
023	CLX	-51	060	-	-45	097	RCL7	36 07	134	RCL1	36 01
024	RCL1	36 01	061	x	-35	098	RCL8	36 08	135	+	-55
025	2	02	062	-	-45	099	-	-45	136	PRTX	-14
026	÷	-24	063	RCLA	36 11	100	x	-35	137	RCLC	36 13
027	RCL4	36 04	064	x	-35	101	RCL1	36 01	138	RCL6	36 06
028	2	02	065	PRTX	-14	102	2	02	139	CHS	-22
029	÷	-24	066	RCL3	36 03	103	÷	-24	140	x	-35
030	-	-45	067	-	-45	104	RCL4	36 04	141	RCL2	36 02
031	RCL0	36 00	068	STOB	35 12	105	2	02	142	+	-55
032	RCL6	36 06	069	CHS	-22	106	÷	-24	143	PRTX	-14
033	x	-35	070	2	02	107	-	-45	144	RTN	24
034	+	-55	071	x	-35	108	RCL0	36 00	145	R/S	51
035	RCL3	36 03	072	RCL8	36 08	109	RCL6	36 06			
036	RCL8	36 08	073	x	-35	110	x	-35			
037	x	-35	074	RCL4	36 04	111	+	-55			

Registers

0	d_4	1	β_4	2	γ_4	3	d_1	4	β_1
5	γ_1	6	ρ_{43}	7	ρ_{32}	8	ρ_{21}	9	$d_2 - d_1$

Table D.1 Program for the matching functions



STEP	INSTRUCTIONS	INPUT DATA/UNITS	KEYS	OUTPUT DATA/UNITS
1	Load side 1 and side 2 of program			
2	Load input data	α_4	STO 0	α_4
		β_4	STO 1	β_4
		γ_4	STO 2	γ_4
		α_1	STO 3	α_1
		β_1	STO 4	β_1
		γ_1	STO 5	γ_1
		ρ_{43}	STO 6	ρ_{43}
		ρ_{32}	STO 7	ρ_{32}
		ρ_{21}	STO 8	ρ_{21}
3	Start the calculation		A	α_2
				β_2
				γ_2
				α_3
				β_3
				γ_3

Table D.2 User instructions
for calculating matching functions

VITA



Name Mr. Wichit Sritrakool

Born October 10 , 1953
Meklong, Samutsongkram

Degree B.Sc. in Physics, April, 1975
Chulalongkorn University
Bangkok, Thailand

Graduate Scholarship University Development Commission
National Education Council
Bangkok
June 1975 - May 1977

Graduate School Assistantship
Chulalongkorn University
Bangkok
August 1977 - November 1977