MANCHESTER UNIVERSITY COMPUTING MACHINE LABORATORY

Programme Sheet B

ROUTINE Orbital Map **Date** March 56.

/	K	/	½	/	
/	/	/	T	£	
E	/	/	T	£	
@	/	/	T	£	
A	/	/	T	£	
:	/	½	Y	0	B5 = 20 } y counters
S	/	½	L	0	B2 = 20 } y counters
I	/	:	P	0	B6 = 0 } x counters
U	/	½	W	0	B3 = 20 } x counters
½	A	/	T	:	A = 0
D	/	R	Y	B	store y
R	@	R	P	B	store x
J	/	R	/	C	D = y
N	:	½	/	N	
F	:	R	T	A	store Y = $\frac{1}{3}(\frac{2}{3}\cdot\frac{y}{64})$
C	@	R	/	C	D = x
K	:	½	/	N	
T	I	R	T	A	store X = $\frac{1}{3}(\frac{2}{3}\cdot\frac{x}{64})$
Z	I	R	/	C	D = X
L	I	R	/	N	A = X^2
W	:	R	/	C	D = Y
H	:	R	/	N	A = X^2+Y^2
Y	R	R	/	U	L = X^2+Y^2
P	/	D	/	J	
Q	Q	/	Q	0	square root → $\frac{1}{3}\cdot\frac{L}{64}$
O	F	S	/	P	
B	R	R	/	S	store $\frac{1}{3}\cdot\frac{L}{64}$ also L = $\frac{1}{3}\cdot\frac{L}{64}$
G	@	R	H	0	B4 = x
,,	E	:	H	G	B4 = x−1
M	½	/	/	0	if +ve → instruction /E
X	D	S	T	/	if −ve, L = £££££££ ≈ 1
V	N	R	T	A	store sin φ = 1
£	I	½	/	Q	→ instruction SE

E	K	/	D	/	
/	:	R	/	C	D = Y (and L already = $\frac{1}{3}\cdot\frac{L}{64}$)
E	@	D	/	J	
@	@	E	Q	0	division → sin φ
A	F	S	/	P	
:	N	R	T	A	store sin φ
S	/	R	H	0	B4 = y
I	E	:	H	G	B4 = y−1
U	½	/	/	0	if +ve → instruction JE
½	D	S	T	/	if −ve, L ≈ 1.
D	C	R	T	A	store cos φ = 1
R	"	E	/	P	→ instruction ZE
J	R	R	T	/	L = $\frac{1}{3}\cdot\frac{L}{64}$
N	I	R	/	C	D = x
F	@	D	/	J	
C	C	E	Q	0	division → cos φ
K	F	S	/	P	
T	C	R	T	A	store cos φ
Z	:	D	T	/	
L	@	/	Z	A	
W	R	R	T	F	L = $\frac{1}{3}\frac{L}{64}$: exponential → $\frac{1}{2}e^{-\frac{1}{3}\cdot\frac{L}{64}}$
H	H	E	Q	0	
Y	K	S	/	P	
P	½	R	T	A	store $\frac{1}{2}e^{-\frac{1}{3}\cdot\frac{L}{64}}$
Q	I	½	H	0	B4 = S
O	½	R	/	C	D = [½R]
B	½	R	/	N	A = $[\frac{1}{2}R]^2$
G	½	R	/	E	store product in ½R
,,	T	E	T	:	A = 0
M	A	:	/	C	D = 2
X	½	R	/	N	A = 2[½R]
V	½	R	T	A	store $\frac{1}{2}e^{-\frac{1}{2}\cdot\frac{L}{62}}$ etc
£	E	:	H	G	1 → B4

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Programme Sheet B

ROUTINE Orbital Map Page 2 (d_{xy} orbital) **Date**

@	K / R /					A	K / J /				
/	V	A	/	T	back to OE if +ve	/	/	/	T	:	
E	R	R	/	C	if -ve	E	C	R	/	C	$D = \cos\phi$
@	R	R	/	N	$A = \frac{1}{9}\cdot\frac{\rho^3}{64^2}$	@	O	R	/	F	$A = \frac{1}{\sqrt{2}}\cdot\frac{1}{4}\cdot\frac{1}{9}\cdot\frac{1}{64^2}\,\psi_p$
A	T	R	/	E	store	A	O	R	/	E	store
:	/	/	T	:		:	/	/	T	:	
S	R	R	/	C		S	L	½	/	C	$D = \frac{\sqrt{2}}{4}$
I	½	½	/	N	$A = \frac{1}{9}\cdot\frac{6\rho}{64^2}$	I	T	R	/	N	$A = \frac{\sqrt{2}}{4}\cdot\frac{1}{9}\cdot\frac{1}{64^2}\cdot\rho^2$
U	V	D	/	U	$L = \frac{1}{9}\cdot\frac{6\rho}{64^2}$	U	Q	R	/	E	store
½	T	R	T	N	$A = \frac{1}{9}\cdot\frac{1}{64^2}(6\rho-\rho^2)$	½	/	/	T	:	
D	L	R	T	A	store and A = 0	D	½	R	/	C	$D = \frac{1}{2}e^{-\rho/3}$
R	R	½	/	J	$M = \frac{1}{9}\cdot\frac{27}{64^2}$	R	Q	R	/	N	$A = \frac{1}{2}\cdot\frac{\sqrt{2}}{4}\cdot\frac{1}{9}\cdot\frac{1}{64^2}\cdot\rho^2 e^{-\rho/3}$
J	N	½	/	C	$D = \frac{1}{3}\cdot\frac{18}{64}$	J	Q	R	/	E	store
N	R	R	/	½	$M = \frac{1}{9}\cdot\frac{1}{64^2}(27-18\rho)$	N	/	/	T	:	
F	T	R	/	J	$M = \frac{1}{9}\cdot\frac{1}{64^2}(27-18\rho+\rho^2)$	F	N	R	/	C	$D = \sin\phi$
C	T	R	/	J	$M = \frac{1}{9}\cdot\frac{1}{64^2}(27-18\rho+2\rho^2)$	C	C	R	/	N	$A = \cos\phi\sin\phi$
K	H	R	/	E	store	K	M	R	/	E	store
T	/	/	T	:		T	/	/	T	:	
Z	C	½	/	C	$D = \frac{1}{4\sqrt{3}}$	Z	M	R	/	C	$D = \cos\phi\sin\phi$
L	H	R	/	F	$A = \frac{1}{4\sqrt{3}}\cdot\frac{1}{9}\cdot\frac{1}{64^2}(27-18\rho+2\rho^2)$	L	Q	R	/	N	$A = \frac{1}{2}\cdot\frac{1}{4}\cdot\frac{1}{9}\cdot\frac{1}{64^2}\,\psi_d$
W	P	R	/	E	store	W	Q	R	/	E	store
H	/	/	T	:		H	/	/	T	:	
Y	½	R	/	C	$D = \frac{1}{2}e^{-\rho/3}$	Y	P	R	T	½	$A = \frac{1}{2}\cdot N\cdot\psi_s$
P	P	R	/	F	$A = \frac{1}{2}\cdot\frac{1}{4}\cdot\frac{1}{9}\cdot\frac{1}{64^2}\cdot\psi_s$	P	O	R	T	C	$A = N\cdot(\frac{1}{2}\psi_s + \frac{1}{\sqrt{2}}\psi_p)$
Q	P	R	/	E	store	Q	Q	R	T	C	$A = N(\frac{1}{2}\psi_s + \frac{1}{\sqrt{2}}\psi_p + \frac{1}{2}\psi_d)$
O	/	/	T	:		O	V	R	T	A	store
B	T	½	/	C	$D = \sqrt{2}\cdot\frac{\sqrt{2}}{4}$	B	I	D	/	J	
G	L	R	/	F	$A = \sqrt{2}\cdot\frac{\sqrt{2}}{4}\cdot\frac{1}{9}\cdot\frac{1}{64^2}(6\rho-\rho^2)$	G	/	/	E	A	
,,	O	R	/	E	store	,,	M	A	/	P	call in print routine
M	/	/	T	:		M	T	S	/	/	
X	½	R	/	C	$D = \frac{1}{2}e^{-\rho/3}$	X	/	/	/	/	control number
V	O	R	/	F	$A = \frac{1}{\sqrt{2}}\cdot\frac{\sqrt{2}}{4}\cdot\frac{1}{9}\cdot\frac{1}{64^2}(6\rho-\rho^2)e^{-\rho/3}$	V	Q	E	/	/	
£	O	R	/	E	store	£	/	/	/	/	control number

M @ I R ½

MANCHESTER UNIVERSITY COMPUTING MACHINE LABORATORY

Programme Sheet B

ROUTINE Orbital Map, Page 2 ($d_{x^2-y^2}$ orbital) **Date** _____

/			A	/					
E				E					
@				@					
A				A					
:				:					
S				S					
I				I					
U				U					
½				½					
D				D					
R				R					
J				J					
N				N	/	/	T	:	
F				F	C	R	/	C	D = cos φ (always < 1)
C				C	C	R	/	N	A = cos² φ (always < 1)
K				K	M	R	/	U	L = cos² φ (MR = wibbish)
T				T	I	S	T	C	L = cos² φ − ½
Z				Z	M	R	T	A	store (cos² φ − ½), A = 0
L				L	M	R	/	K	D = cos² φ − ½
W				W	Q	R	/	F	A = ½ · ¼ · ⅓ · 1/6a₀³ · ψ_d
H				H	Q	R	/	E	store
Y				Y	P	R	T	½	A = ½ · N · ψ_s
P				P	O	R	T	C	A = N · (½ ψ_s + 1/√2 ψ_p)
Q				Q	Q	R	T	C	A = N(½ ψ_s + 1/√2 ψ_p + ½ ψ_d)
O				O	V	R	T	A	store
B				B					
G				G					
,,				,,					
M				M					
X				X					
V				V					
£				£					

MANCHESTER UNIVERSITY COMPUTING MACHINE LABORATORY

Programme Sheet B

ROUTINE Orbital Map, Pointing. **Date**

	K / ½ /					K / D /				
/					E					
/	V	R	T	½	$A = \frac{1}{4}\cdot\frac{1}{9}\cdot\frac{1}{64^2}\cdot\Psi$	/	J	E	/	O	test B3, if +ve → instruction KE
E	E	:	/	M	test sign + if +ve jump one instruction	E	E	:	Y	G	if -ve take 1 off B5
@	V	R	T	F	if -ve, $A = -\frac{1}{4}\cdot\frac{1}{9}\cdot\frac{1}{64^2}\cdot\Psi$	@	E	:	L	G	take 1 off B2
A	M	E	T	N	subtract [ME]	A	E	:	/	O	if +ve, jump one instruction
:	L	E	/	H	if A +ve → instruction LE	:	/	/	/	L	if -ve, stop on L stop.
S	/	/	T	:		S	@	½	/	J	m.s.d. = L
I	H	½	/	C	D = scale factor	I	Y	/	/	:	carriage return
U	V	R	/	F	$A = k\Psi$	U	V	:	/	J	m.s.d. = E + L = W
½	G	/	/	M	if +ve → instruction N1	½	Y	/	/	:	line feed
D	M	R	T	A	if -ve, store	D	D	S	/	J	m.s.d. = £ + W = L
R	M	R	T	F	change sign	R	Y	/	/	:	carriage return
J	I	S	T	I	add 1 in last digit = add 50.	J	C	/	T	:	
N	G	E	T	I	Round off.	N	½	D	/	J	
F	M	R	T	A	store final form of Ψ	F	/	/	E	A	call in orbital routine, entry 1
C	E	:	H	O	B4 = 1	C	O	E	/	P	
K	P	½	/	C	D = 10	K	R	D	/	J	
T	M	R	/	N	$A = 10\Psi$	T	/	/	E	A	call in orbital routine, entry 2
Z	M	R	/	U	store fractional part F	Z	O	E	/	P	
L	V	R	T	A	store integral part I	L	Z	E	T	:	
W	V	:	/	C	$D = 2^{35}$	W	O	½	/	J	m.s.d. = Z
H	V	R	/	N	$A = 2^{35} I$	H	Y	/	/	:	print space
Y	V	R	T	A	store	Y	Y	/	/	:	print space
P	V	R	/	J	m.s.d = I	P	Q	E	/	P	return to instruction M1
Q	Y	/	/	:	print	Q	"	/	/	/	control number
O	E	:	H	G	1 off B4	O	T	S	/	/	
B	X	/	/	T	if +ve → instruction K1	B	/	/	/	/	control number
G	A	/	T	:	if -ve, clear A	G	"	A	S	M	
,,	O	½	/	J	m.s.d. = Z	,,	G	A	S	/	round off constant
M	Y	/	/	:	print space	M	B	Z	A	U	
X	C	/	T	:		X	C	/	/	/	test constant = 49
V	D	S	P	G	add 1 to B6	V					
£	E	:	W	G	take 1 off B3	£					

M E I D ½

MANCHESTER UNIVERSITY COMPUTING MACHINE LABORATORY

Programme Sheet B

ROUTINE Orbital map. constants and transfer cues. **Date** _____

½	K / ½ /	
/	H / / /	20
E	/ / / /	
@	/ / / /	carriage return
A	/ / / L	
:	: U C M	$\frac{1}{3} \cdot \frac{2}{3} \cdot \frac{1}{64}$
S	O Z A /	
I	S / / /	5
U	/ / / /	
½	/ / / /	$\frac{1}{3} \cdot \frac{6}{64}$
D	/ / / E	
R	/ / / /	$\frac{1}{9} \cdot \frac{27}{64^2}$
J	/ O / /	
N	/ / / /	$\frac{1}{3} \cdot \frac{18}{64}$
F	/ / / A	
C	/ E A X	$\frac{1}{4} \cdot \frac{1}{\sqrt{3}}$
K	H B W :	
T	/ / / /	$\frac{1}{4} \cdot \sqrt{2} \times \sqrt{2}$
Z	/ / / T	
L	X K I W	$\frac{1}{4} \cdot \sqrt{2}$
W	U E R J	
H	/ / : E	scale up =
Y	/ / / /	
P	R / / /	10
Q	/ / / /	
O	/ / / /	space
B	/ / / Z	
G		
,,		
M		
X		
V		
£		

D	K / D T	
/	≠ E / /	square root
E	P / E @	
@	≠ E / /	division
A	Y / E @	
:	E @ / /	exponential
S	O / E @	
I	≠ ≠ / /	printing
U	E I E /	
½	S / / /	orbital map, entry 1 (resets $\alpha = 20$)
D	@ I @ /	
R	U / / /	orbital map, entry 2
J	@ I @ /	
N		
F		
C		
K		
T		
Z		
L		
W		
H		
Y		
P		
Q		
O		
B		
G		
,,		
M		
X		
V		
£		

M A I ½ ½

H

Orbital Map Steering Tapes

Run complete program with H stop on once H has been encountered.

1st quadrant:

M	A	I	/	½
	K	H	S	@
	£	£	/	/
	@	I	@	/
T	T	S		

starting sequence

N.B. Fig shift on printer (H)

~~CR (L)~~
~~LF (W)~~ Tape punch
~~CR (L)~~

before starting.

after stopping on final H stop
~~print several spaces (Z)~~

2nd quadrant:

M	@	I	@	½
	K	I	½	E
	/	½	P	O
	K	P	J	@
	O	R	T	N
	Q	R	T	N
M	@	I	R	½
M	E	I	E	½
	K	V	½	E
	E	:	P	Q
M	E	I	D	½

bring map routine to sub 5

start B6 at 20

change signs of ψ_p -ve

change sign of ψ_d -ve

rewrite

bring down print routine

take 1 off B6

rewrite.

clear SS manually
starting sequence

3rd quadrant:

M	@	I	@	½
	K	:	½	E
	/	:	Y	O
	K	P	J	@
	O	R	T	N
	Q	R	T	C
M	@	I	R	½
M	E	I	E	½
	K	E	D	E
	D	S	Y	Q
M	E	I	D	½

start B5 at 0

sign of ψ_p -ve

sign of ψ_d +ve

add 16 B5

clear SS manually
starting sequence.

4th quadrant:

M	@	I	@	½
	K	I	½	E
	/	:	P	O
	K	P	J	@
	O	R	T	C
	Q	R	T	N
M	@	I	R	½

start B6 at 0

sign of ψ_p +ve

sign of ψ_d -ve

M	E	I	E	½
	K	V	½	E
	D	S	P	Q
M	E	I	D	½

add 16 B6.

clear SS manually
starting sequence

Orbital Map Steering Types ($d_{x^2-y^2}$ orbital)

1st quadrant : M A I / ½ steering sequence.
K H S @
£ £ / /
@ I @ /
T T S

2nd quadrant : M @ I @ ½
K I ½ E
/ ½ P O
K P J E
O R T N
M @ I R ½ etc.

3rd quadrant : M @ I @ ½
K : ½ E
// : Y O
K P J E
O R T N
M @ I R ½ etc

4th quadrant : M @ I @ ½
K I ½ E
/ : P O
K P J E
O R T C
M @ I R ½ etc.

MANCHESTER UNIVERSITY COMPUTING MACHINE LABORATORY

Programme Sheet B

ROUTINE Orbital Map Page 2 modified for Slater functions **Date** _____

K / R /

@					
/	V	A	/	T	
E	R	R	/	C	
@	R	R	/	N	
A	T	R	/	E	$[TR] = \frac{1}{9}\cdot\frac{1}{64^2}\cdot\rho^2$
:	/	/	T	:	
S	/	/	T	£	
I	/	/	T	£	
U	/	/	T	£	
½	/	/	T	£	
D	/	/	T	£	
R	/	/	T	£	
J	/	/	T	£	
N	/	/	T	£	
F	/	/	T	£	
C	/	/	T	£	
K	/	/	T	£	
T	/	/	T	£	
Z	C	½	/	C	$D = \frac{1}{4}\sqrt{\frac{2}{15}}$
L	T	R	/	N	$A = \frac{1}{4}\sqrt{\frac{2}{15}}\cdot\frac{1}{4}\cdot\frac{1}{64^2}\cdot\rho^2$
W	P	R	/	E	
H	/	/	T	:	
Y	½	R	/	C	$D = \frac{1}{2}e^{-\rho/3}$
P	P	R	/	N	$A = \frac{1}{2}\cdot\frac{1}{4}\sqrt{\frac{2}{15}}\cdot\frac{1}{4}\cdot\frac{1}{64^2}\cdot\rho^2 e^{-\rho/3}$
Q	P	R	/	E	$= \frac{1}{2}\cdot\frac{1}{4}\cdot\frac{1}{4}\cdot\frac{1}{64^2}\cdot\psi_3'$
O	/	/	T	:	
B	T	½	/	C	$D = \sqrt{2}\cdot\frac{1}{4}\cdot\sqrt{\frac{2}{5}}$
G	T	R	/	N	$A = \sqrt{2}\cdot\frac{1}{4}\cdot\sqrt{\frac{2}{5}}\cdot\frac{1}{4}\cdot\frac{1}{64^2}\cdot\rho^2$
,,	O	R	/	E	
M	/	/	T	:	
X	½	R	/	C	$D = \frac{1}{2}e^{-\rho/3}$
V	O	R	/	N	$A = \frac{1}{\sqrt{2}}\cdot\frac{1}{4}\sqrt{\frac{2}{5}}\cdot\frac{1}{4}\cdot\frac{1}{64^2}\cdot\rho^2 e^{-\rho/3}$
£	O	R	/	E	

A					
/	/	/	T	:	
E	C	R	/	C	$D = \cos\phi$
@	O	R	/	N	$A = \frac{1}{12}\cdot\frac{1}{4}\cdot\frac{1}{4}\cdot\frac{1}{64^2}\cdot\psi_\rho'$
A	O	R	/	E	
:	/	/	T	:	
S	etc				
I					
U					
½					
D					
R					
J					
N					
F					
C					
K					
T					
Z					
L					
W					
H					
Y					
P					
Q					
O					
B					
G					
,,					
M					
X					
V					
£					

Rerun main tape, then corrections:

M @ I @ ½
K S R ,,
instructions SR - £R
K @ J E
O R / N
M @ I R ½

M A I / ½
K C ½ :
F H Z C $\frac{1}{4}\cdot\sqrt{\frac{2}{15}}$
D K X @
Q X @ Q $\sqrt{2}\cdot\frac{1}{4}\sqrt{\frac{2}{5}}$
: £ : U
M A I ½ ½

MANCHESTER UNIVERSITY COMPUTING MACHINE LABORATORY

Programme Sheet 2 (b)

ROUTINE *Orbital Map*

	R
/ E	y
@ A	x
: S	Y
I U	X
½ D	$\frac{1}{2} e^{-\frac{1}{3} \cdot \frac{\rho}{64}}$ etc $\rightarrow \frac{1}{2} e^{-\rho/3}$
R J	Dump, $\frac{1}{3} \cdot \frac{\rho}{64}$
N F	$\sin \phi$
C K	$\cos \phi$
T Z	$\frac{1}{9} \cdot \frac{\rho^2}{64^2}$
L W	$\frac{1}{9} \cdot \frac{1}{64^2} (6\rho - \rho^2)$
H Y	$\frac{1}{9} \cdot \frac{1}{64^2} (27 - 18\rho + 2\rho^2)$
P Q	$\frac{1}{2} \cdot \frac{1}{4} \cdot \frac{1}{9} \cdot \frac{1}{64^2} \cdot \psi_s$
O B	$\frac{1}{\sqrt{2}} \cdot \frac{1}{4} \cdot \frac{1}{9} \cdot \frac{1}{64^2} \cdot \psi_p$
G "	$\frac{1}{2} \cdot \frac{1}{4} \cdot \frac{1}{9} \cdot \frac{1}{64^2} \psi_d$
M X	$\cos \phi \sin \phi$, Dump
V £	$\frac{1}{4} \cdot \frac{1}{9} \cdot \frac{1}{64^2} \cdot \Psi$, Dump.