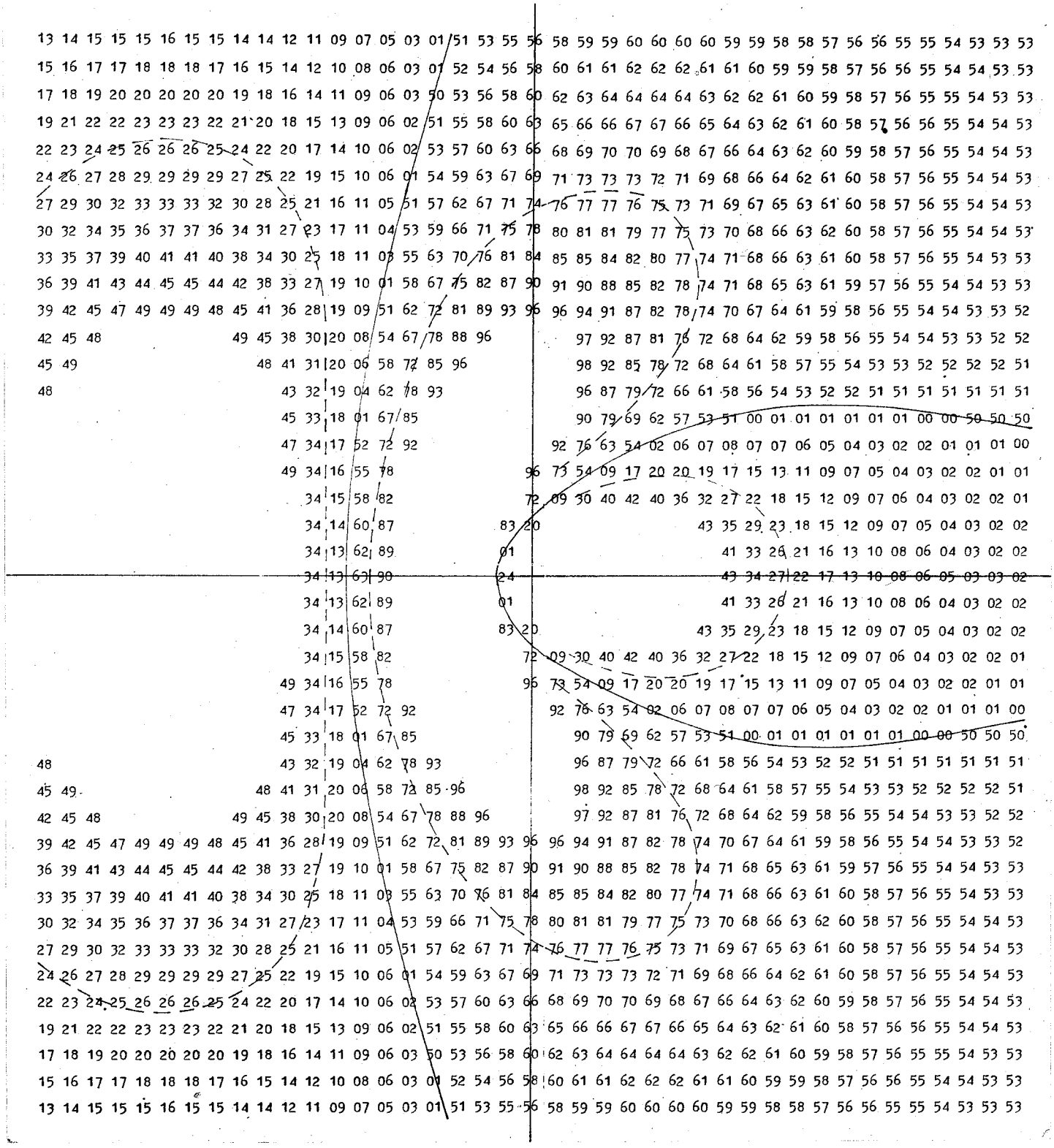
Legend to Figure I.

Contour maps of $\psi = \frac{1}{2}\underline{s} + \frac{1}{2}\underline{d}_{x^2-y^2} + (2)^{-\frac{1}{2}}\underline{p}_x$ using (a) hydrogen-like and (b) Slater 3s, 3p and 3d orbitals covering the area $-\frac{40a_0}{3Z} \leq x,y \leq \frac{40a_0}{3Z}$. A scale factor (the same in both cases) is applied so that in general $-100 \leq \psi \leq 100$. But for the purposes of pictorial representation of both positive and negative magnitudes the value ψ is only printed if $0 \leq |\psi| < 49.5$ and a space is left if $|\psi| \geq 49.5$. Thus the numbers 00 to 49 represent positive values of ψ and the numbers 50 to 99 represeent the corresponding negative values (i.e.17 means $n\psi = 17$, 71 means $n\psi = -21$ and a space means $n|\psi| \geq 49.5$, the sign being obvious from the local environment). These calculations were performed using the Manchester University Electronic Computer.

$\frac{-40a_0}{3Z} \leq x,y \leq \frac{40a_0}{3Z}$

$3sp^2d$ hybrid orbital
(hydrogen-like)



$3sp^2d$ hybrid orbital
(Slater)

52 53 53 54 54 55 56 56 57 58 59 60 60 61 61 62 62 61 61 60 59 58 56 55 53 51 01 02 04 05 07 08 08 09 09 09 09 09 09 09 08
52 53 53 54 55 55 56 57 58 59 60 61 62 62 63 63 63 63 62 61 60 59 57 55 53 51 01 03 05 07 08 09 10 11 11 11 11 11 11 10 10
52 53 53 54 55 56 57 58 59 60 61 62 63 64 64 65 65 64 64 63 61 59 57 55 53 50 02 05 07 09 10 12 13 13 13 14 13 13 13 12 11
52 53 53 54 55 56 57 58 59 60 62 63 64 65 66 66 67 66 65 64 63 60 58 55 52 01 04 06 09 11 13 14 15 16 16 16 16 15 15 14 13
52 53 53 54 55 56 57 58 60 61 63 64 65 67 68 68 68 68 67 66 64 61 58 55 52 02 05 09 11 14 16 17 18 19 19 19 19 18 17 16 15
52 53 53 54 55 56 57 59 60 62 63 65 67 68 69 70 70 70 69 68 65 62 59 55 51 03 07 11 14 17 19 21 22 23 23 22 22 21 20 18 17
52 52 53 54 55 56 57 59 60 62 64 66 68 69 71 72 72 72 71 69 67 63 59 54 00 05 10 14 18 21 24 25 26 27 27 26 25 24 23 21 20
52 52 53 54 54 56 57 58 60 62 64 66 68 70 72 73 74 74 73 71 68 64 59 54 02 08 13 18 22 26 28 30 31 31 31 30 29 28 26 24 22
51 52 52 53 54 55 56 58 60 62 64 66 69 71 73 75 76 76 75 73 69 64 59 52 04 11 17 23 28 31 34 36 37 37 36 35 33 31 29 27 25
51 51 52 52 53 54 56 57 59 61 64 66 69 72 74 76 77 77 76 74 70 65 58 50 07 15 22 28 34 38 41 42 43 43 42 40 38 36 33 30 28
50 51 51 52 52 54 55 56 58 60 63 66 68 71 74 77 78 79 78 75 71 64 57 02 11 20 28 35 41 45 48 49 49 48 45 43 40 37 34 31
00 00 50 51 51 52 54 55 57 59 61 64 67 71 74 76 79 79 79 78 71 64 55 05 15 25 35 42 49 48 44 41 37 34
01 01 01 00 50 51 52 53 55 57 59 62 65 69 72 75 78 79 79 76 71 63 53 09 21 32 42 49 45 41 37
02 02 01 01 01 00 50 52 53 55 57 60 63 66 70 73 76 78 78 75 70 61 01 14 27 40 49 44 40
02 02 02 02 02 02 01 01 51 52 54 56 59 63 66 70 73 76 76 74 68 58 04 19 34 48 47 42
03 03 03 03 03 03 03 03 02 01 51 53 55 58 62 65 69 72 73 72 66 55 09 25 42 45
03 04 04 04 05 05 05 05 04 04 03 01 51 53 56 60 64 67 69 68 62 52 14 32 47
04 04 05 05 06 06 06 07 07 06 06 05 04 02 51 54 57 60 63 63 59 02 19 39 49
04 05 05 06 07 07 08 08 08 09 08 08 07 06 04 02 50 53 56 58 55 06 24 45
05 05 06 06 07 08 08 09 09 10 10 10 10 09 08 07 05 02 50 52 52 08 27 49
05 05 06 07 07 08 09 09 10 10 11 11 11 10 09 08 06 05 03 01 00 09 28
05 05 06 06 07 08 08 09 09 10 10 10 10 09 08 07 05 02 50 52 52 08 27 49
04 05 05 06 07 07 08 08 08 09 08 08 07 06 04 02 50 53 56 58 55 06 24 45
04 04 05 05 06 06 06 07 07 06 06 05 04 02 51 54 57 60 63 63 59 02 19 39 49
03 04 04 04 05 05 05 05 04 04 03 01 51 53 56 60 64 67 69 68 62 52 14 32 47
03 03 03 03 03 03 03 03 02 01 51 53 55 58 62 65 69 72 73 72 66 55 09 25 42 45
02 02 02 02 02 02 01 01 51 52 54 56 59 63 66 70 73 76 76 74 68 58 04 19 34 48 47 42
02 02 01 01 01 00 50 52 53 55 57 60 63 66 70 73 76 78 78 75 70 61 01 14 27 40 49 44 40
01 01 01 00 50 51 52 53 55 57 59 62 65 69 72 75 78 79 79 76 71 63 53 09 21 32 42 49 45 41 37
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50 51 51 52 52 54 55 56 58 60 63 66 68 71 74 77 78 79 78 75 71 64 57 02 11 20 28 35 41 45 48 49 49 48 45 43 40 37 34 31
51 51 52 52 53 54 56 57 59 61 64 66 69 72 74 76 77 77 76 74 70 65 58 50 07 15 22 28 34 38 41 42 43 43 42 40 38 36 33 30 28
51 52 52 53 54 55 56 58 60 62 64 66 69 71 73 75 76 76 75 73 69 64 59 52 04 11 17 23 28 31 34 36 37 37 36 35 33 31 29 27 25
52 52 53 54 54 56 57 58 60 62 64 66 68 70 72 73 74 74 73 71 68 64 59 54 02 08 13 18 22 26 28 30 31 31 31 30 29 28 26 24 22
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52 53 53 54 55 56 57 58 60 61 63 64 65 67 68 68 68 68 67 66 64 61 58 55 52 02 05 09 11 14 16 17 18 19 19 19 19 18 17 16 15
52 53 53 54 55 56 57 58 59 60 62 63 64 65 66 66 67 66 65 64 63 60 58 55 52 01 04 06 09 11 13 14 15 16 16 16 16 15 15 14 13
52 53 53 54 55 56 57 58 59 60 61 62 63 64 64 65 65 64 64 63 61 59 57 55 53 50 02 05 07 09 10 12 13 13 13 14 13 13 13 12 11
52 53 53 54 55 55 56 57 58 59 60 61 62 62 63 63 63 63 62 61 60 59 57 55 53 51 01 03 05 07 08 09 10 11 11 11 11 11 11 10 10
52 53 53 54 54 55 56 56 57 58 59 60 60 61 61 62 62 61 61 60 59 58 56 55 53 51 01 02 04 05 07 08 08 09 09 09 09 09 09 09 08