Contents

1 Hamiltonian

Hamiltonian of the atom

$$\mathcal{H} = \sum 5.0 V_{e-e} \tag{1}$$

Number of electrons in the d shell = 2
Lower case l, s denote single particle operators
Upper case L, S, J denote multi particle operators

2 Spectrum

There are 45 different states
There are 5 different manifolds

Manifold	Degeneracy	ΔE (eV)	Energy (eV)
GS	21	0.000	0.000
Excited #1	5	3.424	3.424
Excited #2	9	3.965	3.965
Excited #3	9	5.275	5.275
Excited #4	1	13.175	13.175

3 Eigenstates and expectation values

Energy (GHz)	Energy (meV)	L_x	L_y	L_z	S_x	S_y	S_z
0.000	0.000	0.000	0.000	0.000	0.000	0.000	-1.000
0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.000
0.000	0.000	-0.000	0.000	-0.000	-0.000	0.000	-0.000
0.000	0.000	0.000	0.000	-2.000	0.000	0.000	-0.000
0.000	0.000	0.000	0.000	1.948	-0.000	0.000	-0.013
0.000	0.000	0.000	0.000	2.000	0.000	0.000	1.000
0.000	0.000	0.000	0.000	-2.000	0.000	0.000	1.000
0.000	0.000	-0.000	0.000	-1.948	-0.000	0.000	-0.987
0.000	0.000	0.000	0.000	2.000	0.000	0.000	-1.000
0.000	0.000	0.000	0.000	3.000	0.000	0.000	1.000
0.000	0.000	0.000	0.000	-3.000	0.000	0.000	1.000
0.000	0.000	0.000	0.000	3.000	0.000	0.000	-1.000
0.000	0.000	-0.000	0.000	-3.000	0.000	0.000	-1.000
0.000	0.000	-0.000	0.000	3.000	0.000	0.000	-0.000
0.000	0.000	0.000	0.000	-3.000	0.000	0.000	0.000
0.000	0.000	-0.000	0.000	0.989	0.001	0.000	-1.000
0.000	0.000	-0.000	0.000	-1.000	-0.000	0.000	-0.000
0.000	0.000	0.000	0.000	1.000	0.000	0.000	1.000
0.000	0.000	0.000	0.000	-0.987	-0.003	0.000	-0.999
0.000	0.000	0.000	0.000	-1.000	0.000	0.000	1.000
0.000	0.000	-0.000	0.000	0.998	0.002	0.000	-0.001
828053.204	3424.000	0.000	0.000	-0.000	0.000	0.000	-0.000
828053.204	3424.000	-0.000	0.000	-2.000	0.000	0.000	-0.000
828053.204	3424.000	-0.000	0.000	2.000	-0.000	0.000	-0.000
828053.204	3424.000	0.000	0.000	-1.000	-0.000	0.000	-0.000
828053.204	3424.000	0.000	0.000	1.000	-0.000	0.000	-0.000
958887.545	3965.000	-0.000	0.000	0.000	0.000	0.000	-0.000
958887.545	3965.000	0.000	0.000	0.000	0.000	0.000	1.000
958887.545	3965.000	-0.000	0.000	0.000	-0.000	0.000	-1.000
958887.545	3965.000	0.000	0.000	-1.000	0.000	0.000	1.000
958887.545	3965.000	0.000	0.000	1.000	0.000	0.000	-1.000
958887.545	3965.000	0.000	0.000	-1.000	-0.000	0.000	-0.000
958887.545	3965.000	0.000	0.000	-1.000	0.000	0.000	-1.000
958887.545	3965.000	-0.000	0.000	1.000	0.000	0.000	1.000
958887.545	3965.000	0.000	0.000	1.000	-0.000	0.000	-0.000
1275695.284	5275.000	0.000	0.000	4.000	0.000	0.000	-0.000

Energy (GHz)	Energy (meV)	L_x	L_y	L_z	S_x	S_y	S_z
1275695.284	5275.000	0.000	0.000	-4.000	0.000	0.000	0.000
1275695.284	5275.000	-0.000	0.000	-0.000	-0.000	0.000	-0.000
1275695.284	5275.000	0.000	0.000	-2.000	-0.000	0.000	-0.000
1275695.284	5275.000	-0.000	0.000	2.000	-0.000	0.000	-0.000
1275695.284	5275.000	0.000	0.000	-3.000	0.000	0.000	0.000
1275695.284	5275.000	0.000	0.000	3.000	0.000	0.000	-0.000
1275695.284	5275.000	0.000	0.000	1.000	0.000	0.000	-0.000
1275695.284	5275.000	-0.000	0.000	-1.000	-0.000	0.000	-0.000
3186215.236	13175.000	0.000	0.000	-0.000	0.000	0.000	-0.000

4 Proyection of operator on GS

Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large.. Matrix too large..

5 Wavefunctions

5.1 Ground state manifold

$$\Psi_1 = \begin{pmatrix} & |-2\downarrow,-1\downarrow\rangle \end{pmatrix} \tag{2}$$

$$\Psi_2 = \begin{pmatrix} \frac{1}{\sqrt{2}} & |-1\uparrow,-2\downarrow\rangle \\ -\frac{1}{\sqrt{2}} & |-2\uparrow,-1\downarrow\rangle \end{pmatrix} \tag{3}$$

$$\Psi_3 = \begin{pmatrix} & |-2\downarrow,0\downarrow\rangle \end{pmatrix} \tag{4}$$

$$\Psi_4 = \begin{pmatrix} & |-2\uparrow,-1\uparrow\rangle \end{pmatrix} \tag{5}$$

$$\Psi_5 = \begin{pmatrix} -\frac{1}{\sqrt{2}} & |0\uparrow,-2\downarrow\rangle \\ \frac{1}{\sqrt{2}} & |-2\uparrow,0\downarrow\rangle \end{pmatrix} \tag{6}$$

$$\Psi_6 = \begin{pmatrix} 0.77 & |-2\downarrow,+1\downarrow\rangle \\ 0.63 & |-1\downarrow,0\downarrow\rangle \end{pmatrix} \tag{7}$$

$$\Psi_7 = \begin{pmatrix} 0.55 & |-2\uparrow,+1\downarrow\rangle \\ -0.55 & |+1\uparrow,-2\downarrow\rangle \\ 0.45 & |-1\uparrow,0\downarrow\rangle \\ -0.45 & |0\uparrow,-1\downarrow\rangle \end{pmatrix} \tag{8}$$

$$\Psi_8 = \begin{pmatrix} 0.89 & |-1\downarrow,+1\downarrow\rangle \\ 0.45 & |-2\downarrow,+2\downarrow\rangle \end{pmatrix} \tag{9}$$

$$\Psi_9 = \begin{pmatrix} & |-2\uparrow, 0\uparrow\rangle \end{pmatrix} \tag{10}$$

$$\Psi_{10} = \begin{pmatrix} -0.77 & |-1\downarrow, +2\downarrow\rangle \\ -0.63 & |0\downarrow, +1\downarrow\rangle \end{pmatrix} \tag{11}$$

$$\Psi_{11} = \begin{pmatrix} 0.77 & |-2\uparrow, +1\uparrow\rangle \\ 0.63 & |-1\uparrow, 0\uparrow\rangle \end{pmatrix} \tag{12}$$

$$\Psi_{12} = \begin{pmatrix} 0.63 & |-1\uparrow, +1\downarrow\rangle \\ -0.63 & |+1\uparrow, -1\downarrow\rangle \\ -0.32 & |+2\uparrow, -2\downarrow\rangle \\ 0.32 & |-2\uparrow, +2\downarrow\rangle \end{pmatrix} \tag{13}$$

$$\Psi_{13} = \begin{pmatrix} & |0\downarrow, +2\downarrow\rangle \end{pmatrix} \tag{14}$$

$$\Psi_{14} = \begin{pmatrix} -0.55 & |+2\uparrow, -1\downarrow\rangle \\ 0.55 & |-1\uparrow, +2\downarrow\rangle \\ 0.45 & |0\uparrow, +1\downarrow\rangle \\ -0.45 & |+1\uparrow, 0\downarrow\rangle \end{pmatrix} \tag{15}$$

$$\Psi_{15} = \begin{pmatrix} -0.89 & |-1\uparrow, +1\uparrow\rangle \\ -0.45 & |-2\uparrow, +2\uparrow\rangle \end{pmatrix} \tag{16}$$

$$\Psi_{16} = \begin{pmatrix} & |+1\downarrow, +2\downarrow\rangle \end{pmatrix} \tag{17}$$

$$\Psi_{17} = \begin{pmatrix} 0.77 & |-1\uparrow, +2\uparrow\rangle \\ 0.63 & |0\uparrow, +1\uparrow\rangle \end{pmatrix} \tag{18}$$

$$\Psi_{18} = \begin{pmatrix} -\frac{1}{\sqrt{2}} & |0\uparrow, +2\downarrow\rangle \\ \frac{1}{\sqrt{2}} & |+2\uparrow, 0\downarrow\rangle \end{pmatrix} \tag{19}$$

$$\Psi_{19} = \begin{pmatrix} & |0\uparrow, +2\uparrow\rangle \end{pmatrix} \tag{20}$$

$$\Psi_{20} = \begin{pmatrix} -\frac{1}{\sqrt{2}} & |+2\uparrow, +1\downarrow\rangle \\ \frac{1}{\sqrt{2}} & |+1\uparrow, +2\downarrow\rangle \end{pmatrix} \tag{21}$$

$$\Psi_{21} = \begin{pmatrix} & |+1\uparrow, +2\uparrow\rangle \end{pmatrix} \tag{22}$$

5.2 Excited state manifold #1

$$\Psi_1 = \begin{pmatrix} -0.65 & |-1\uparrow,-1\downarrow\rangle \\ 0.53 & |-2\uparrow,0\downarrow\rangle \\ 0.53 & |0\uparrow,-2\downarrow\rangle \end{pmatrix} \tag{23}$$

$$\Psi_2 = \begin{pmatrix} -0.65 & |+1\uparrow,-2\downarrow\rangle \\ -0.65 & |-2\uparrow,+1\downarrow\rangle \\ 0.27 & |0\uparrow,-1\downarrow\rangle \\ 0.27 & |-1\uparrow,0\downarrow\rangle \end{pmatrix} \tag{24}$$

$$\Psi_3 = \begin{pmatrix} 0.53 & |0\uparrow,0\downarrow\rangle \\ -0.53 & |+2\uparrow,-2\downarrow\rangle \\ -0.53 & |-2\uparrow,+2\downarrow\rangle \\ -0.27 & |-1\uparrow,+1\downarrow\rangle \\ -0.27 & |+1\uparrow,-1\downarrow\rangle \end{pmatrix} \tag{25}$$

$$\Psi_4 = \begin{pmatrix} -0.65 & |-1\uparrow,+2\downarrow\rangle \\ -0.65 & |+2\uparrow,-1\downarrow\rangle \\ 0.27 & |0\uparrow,+1\downarrow\rangle \\ 0.27 & |+1\uparrow,0\downarrow\rangle \end{pmatrix} \tag{26}$$

$$\Psi_5 = \begin{pmatrix} -0.65 & |+1\uparrow,+1\downarrow\rangle \\ 0.53 & |+2\uparrow,0\downarrow\rangle \\ 0.53 & |0\uparrow,+2\downarrow\rangle \end{pmatrix} \tag{27}$$

5.3 Excited state manifold #2

$$\Psi_1 = \begin{pmatrix} -0.77 & |-1\downarrow,0\downarrow\rangle \\ 0.63 & |-2\downarrow,+1\downarrow\rangle \end{pmatrix} \tag{28}$$

$$\Psi_2 = \begin{pmatrix} 0.55 & |0\uparrow,-1\downarrow\rangle \\ -0.55 & |-1\uparrow,0\downarrow\rangle \\ 0.45 & |-2\uparrow,+1\downarrow\rangle \\ -0.45 & |+1\uparrow,-2\downarrow\rangle \end{pmatrix} \tag{29}$$

$$\Psi_3 = \begin{pmatrix} -0.89 & |-2\downarrow,+2\downarrow\rangle \\ 0.45 & |-1\downarrow,+1\downarrow\rangle \end{pmatrix} \tag{30}$$

$$\Psi_4 = \begin{pmatrix} 0.77 & |0\downarrow,+1\downarrow\rangle \\ -0.63 & |-1\downarrow,+2\downarrow\rangle \end{pmatrix} \tag{31}$$

$$\Psi_5 = \begin{pmatrix} 0.63 & |-2\uparrow,+2\downarrow\rangle \\ -0.63 & |+2\uparrow,-2\downarrow\rangle \\ 0.32 & |+1\uparrow,-1\downarrow\rangle \\ -0.32 & |-1\uparrow,+1\downarrow\rangle \end{pmatrix} \tag{32}$$

$$\Psi_6 = \begin{pmatrix} -0.77 & |-1\uparrow,0\uparrow\rangle \\ 0.63 & |-2\uparrow,+1\uparrow\rangle \end{pmatrix} \tag{33}$$

$$\Psi_7 = \begin{pmatrix} -0.89 & |-2\uparrow,+2\uparrow\rangle \\ 0.45 & |-1\uparrow,+1\uparrow\rangle \end{pmatrix} \tag{34}$$

$$\Psi_8 = \begin{pmatrix} -0.55 & |0\uparrow,+1\downarrow\rangle \\ 0.55 & |+1\uparrow,0\downarrow\rangle \\ -0.45 & |+2\uparrow,-1\downarrow\rangle \\ 0.45 & |-1\uparrow,+2\downarrow\rangle \end{pmatrix} \tag{35}$$

$$\Psi_9 = \begin{pmatrix} -0.77 & |0\uparrow,+1\uparrow\rangle \\ 0.63 & |-1\uparrow,+2\uparrow\rangle \end{pmatrix} \tag{36}$$

5.4 Excited state manifold #3

$$\Psi_1 = \begin{pmatrix} & |-2\uparrow,-2\downarrow\rangle \end{pmatrix} \tag{37}$$

$$\Psi_2 = \begin{pmatrix} \frac{1}{\sqrt{2}} & |-2\uparrow,-1\downarrow\rangle \\ \frac{1}{\sqrt{2}} & |-1\uparrow,-2\downarrow\rangle \end{pmatrix} \tag{38}$$

$$\Psi_3 = \begin{pmatrix} 0.76 & |-1\uparrow,-1\downarrow\rangle \\ 0.46 & |-2\uparrow,0\downarrow\rangle \\ 0.46 & |0\uparrow,-2\downarrow\rangle \end{pmatrix} \tag{39}$$

$$\Psi_4 = \begin{pmatrix} -0.65 & |-1\uparrow,0\downarrow\rangle \\ -0.65 & |0\uparrow,-1\downarrow\rangle \\ -0.27 & |+1\uparrow,-2\downarrow\rangle \\ -0.27 & |-2\uparrow,+1\downarrow\rangle \end{pmatrix} \tag{40}$$

$$\Psi_5 = \begin{pmatrix} -0.72 & |0\uparrow,0\downarrow\rangle \\ -0.48 & |+1\uparrow,-1\downarrow\rangle \\ -0.48 & |-1\uparrow,+1\downarrow\rangle \\ -0.12 & |-2\uparrow,+2\downarrow\rangle \\ -0.12 & |+2\uparrow,-2\downarrow\rangle \end{pmatrix} \tag{41}$$

$$\Psi_6 = \begin{pmatrix} 0.65 & |+1\uparrow,0\downarrow\rangle \\ 0.65 & |0\uparrow,+1\downarrow\rangle \\ 0.27 & |-1\uparrow,+2\downarrow\rangle \\ 0.27 & |+2\uparrow,-1\downarrow\rangle \end{pmatrix} \tag{42}$$

$$\Psi_7 = \begin{pmatrix} 0.76 & |+1\uparrow,+1\downarrow\rangle \\ 0.46 & |+2\uparrow,0\downarrow\rangle \\ 0.46 & |0\uparrow,+2\downarrow\rangle \end{pmatrix} \tag{43}$$

$$\Psi_8 = \begin{pmatrix} \frac{1}{\sqrt{2}} & |+1\uparrow,+2\downarrow\rangle \\ \frac{1}{\sqrt{2}} & |+2\uparrow,+1\downarrow\rangle \end{pmatrix} \tag{44}$$

$$\Psi_9 = \begin{pmatrix} & |+2\uparrow,+2\downarrow\rangle \end{pmatrix} \tag{45}$$

5.5 Excited state manifold #4

$$\Psi_1 = \begin{pmatrix} 0.45 & |+1\uparrow,-1\downarrow\rangle \\ 0.45 & |-1\uparrow,+1\downarrow\rangle \\ -0.45 & |-2\uparrow,+2\downarrow\rangle \\ -0.45 & |+2\uparrow,-2\downarrow\rangle \\ -0.45 & |0\uparrow,0\downarrow\rangle \end{pmatrix} \tag{46}$$