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## 1 Hamiltonian

Hamiltonian of the atom

$$\mathcal{H} = \sum 4.0V_{e-e} \quad (1)$$

Number of electrons in the d shell = 1

Lower case  $l, s$  denote single particle operators

Upper case  $L, S, J$  denote multi particle operators

## 2 Spectrum

There are 10 different states

There are 1 different manifolds

Manifold	Degeneracy	$\Delta E$ (eV)	Energy (eV)
GS	10	0.000	0.000

## 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	-2.000	0.000	0.000	0.500
0.000	0.000	0.000	0.000	-1.000	0.000	0.000	0.500
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.500
0.000	0.000	0.000	0.000	1.000	0.000	0.000	0.500
0.000	0.000	0.000	0.000	2.000	0.000	0.000	0.500
0.000	0.000	0.000	0.000	-2.000	0.000	0.000	-0.500
0.000	0.000	0.000	0.000	-1.000	0.000	0.000	-0.500
0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.500
0.000	0.000	0.000	0.000	1.000	0.000	0.000	-0.500
0.000	0.000	0.000	0.000	2.000	0.000	0.000	-0.500

## 4 Projection of operator on GS

[illegible]

$$S_y = \begin{pmatrix} 0 & \frac{1}{2}i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{2}i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}i & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2}i & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2}i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2}i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2}i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2}i \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2}i & 0 \end{pmatrix} \quad (3)$$

[illegible]

[illegible]

$$L_x = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \quad (6)$$

$$L_y = \begin{pmatrix} 0 & 0 & 1i & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1i & 0 & 0 & 0 & 0 & 0 & 0 \\ -1i & 0 & 0 & 0 & \sqrt{\frac{3}{2}}i & 0 & 0 & 0 & 0 & 0 \\ 0 & -1i & 0 & 0 & 0 & \sqrt{\frac{3}{2}}i & 0 & 0 & 0 & 0 \\ 0 & 0 & -\sqrt{\frac{3}{2}}i & 0 & 0 & 0 & \sqrt{\frac{3}{2}}i & 0 & 0 & 0 \\ 0 & 0 & 0 & -\sqrt{\frac{3}{2}}i & 0 & 0 & 0 & \sqrt{\frac{3}{2}}i & 0 & 0 \\ 0 & 0 & 0 & 0 & -\sqrt{\frac{3}{2}}i & 0 & 0 & 0 & 1i & 0 \\ 0 & 0 & 0 & 0 & 0 & -\sqrt{\frac{3}{2}}i & 0 & 0 & 0 & 1i \\ 0 & 0 & 0 & 0 & 0 & 0 & -1i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1i & 0 & 0 \end{pmatrix} \quad (7)$$

$$L_z = \begin{pmatrix} -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix} \quad (8)$$

$$L^2 = \begin{pmatrix} 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 \end{pmatrix} \quad (9)$$

$$J_x = \begin{pmatrix} 0 & \frac{1}{2} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & \frac{1}{2} & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & \frac{1}{2} & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & \frac{1}{2} & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{\frac{3}{2}} & \frac{1}{2} & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & \frac{1}{2} & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & \frac{1}{2} & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & \frac{1}{2} & 0 & 0 \end{pmatrix} \quad (10)$$

$$J_y = \begin{pmatrix} 0 & \frac{1}{2}i & 1i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{2}i & 0 & 0 & 1i & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1i & 0 & 0 & \frac{1}{2}i & \sqrt{\frac{3}{2}}i & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1i & -\frac{1}{2}i & 0 & 0 & \sqrt{\frac{3}{2}}i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\sqrt{\frac{3}{2}}i & 0 & 0 & \frac{1}{2}i & \sqrt{\frac{3}{2}}i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\sqrt{\frac{3}{2}}i & -\frac{1}{2}i & 0 & 0 & \sqrt{\frac{3}{2}}i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\sqrt{\frac{3}{2}}i & 0 & 0 & \frac{1}{2}i & 1i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\sqrt{\frac{3}{2}}i & -\frac{1}{2}i & 0 & 0 & 1i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1i & 0 & 0 & \frac{1}{2}i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1i & -\frac{1}{2}i & 0 & 0 \end{pmatrix} \quad (11)$$

$$J_z = \begin{pmatrix} -\frac{5}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{3}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{3}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{5}{2} \end{pmatrix} \quad (12)$$

$$J^2 = \begin{pmatrix} 8.75 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4.75 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 7.75 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 5.75 & \sqrt{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{6} & 6.75 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6.75 & \sqrt{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{6} & 5.75 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 7.75 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 4.75 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8.75 \end{pmatrix} \quad (13)$$

$$\sum l_x^2 = \begin{pmatrix} 1 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{5}{2} & 0 & 0 & 0 & \frac{3}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{5}{2} & 0 & 0 & 0 & \frac{3}{2} & 0 & 0 \\ \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 3 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 \\ 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 3 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} \\ 0 & 0 & \frac{3}{2} & 0 & 0 & 0 & \frac{5}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3}{2} & 0 & 0 & 0 & \frac{5}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 1 \end{pmatrix} \quad (14)$$

$$\sum l_y^2 = \begin{pmatrix} 1 & 0 & 0 & 0 & -\sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -\sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{5}{2} & 0 & 0 & 0 & -\frac{3}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{5}{2} & 0 & 0 & 0 & -\frac{3}{2} & 0 & 0 \\ -\sqrt{\frac{3}{2}} & 0 & 0 & 0 & 3 & 0 & 0 & 0 & -\sqrt{\frac{3}{2}} & 0 \\ 0 & -\sqrt{\frac{3}{2}} & 0 & 0 & 0 & 3 & 0 & 0 & 0 & -\sqrt{\frac{3}{2}} \\ 0 & 0 & -\frac{3}{2} & 0 & 0 & 0 & \frac{5}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{3}{2} & 0 & 0 & 0 & \frac{5}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\sqrt{\frac{3}{2}} & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\sqrt{\frac{3}{2}} & 0 & 0 & 0 & 1 \end{pmatrix} \quad (15)$$

$$\sum l_z^2 = \begin{pmatrix} 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 \end{pmatrix} \quad (16)$$

$$\sum l_x^4 + l_y^4 + l_z^4 = \begin{pmatrix} 21 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 21 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \\ 0 & 0 & 18 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 18 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 24 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 24 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 18 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 18 & 0 & 0 \\ 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 21 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 21 \end{pmatrix} \quad (17)$$

$$V_{e-e} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (18)$$

$$\sum \vec{l} \cdot \vec{s} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (19)$$

## 5 Wavefunctions

### 5.1 Ground state manifold

$$\Psi_1 = ( \quad | -2 \downarrow \rangle ) \quad (20)$$

$$\Psi_2 = ( \quad | -2 \uparrow \rangle ) \quad (21)$$

$$\Psi_3 = ( \quad | -1 \downarrow \rangle ) \quad (22)$$

$$\Psi_4 = ( \quad | -1 \uparrow \rangle ) \quad (23)$$

$$\Psi_5 = ( \quad | 0 \downarrow \rangle ) \quad (24)$$

$$\Psi_6 = ( \quad | 0 \uparrow \rangle ) \quad (25)$$

$$\Psi_7 = ( \quad | +1 \downarrow \rangle ) \quad (26)$$

$$\Psi_8 = ( \quad | + 1 \uparrow \rangle ) \quad (27)$$

$$\Psi_9 = ( \quad | + 2 \downarrow \rangle ) \quad (28)$$

$$\Psi_{10} = ( \quad | + 2 \uparrow \rangle ) \quad (29)$$