

Addition of angular momentum

Let \mathbf{J} be the sum of orbital angular momentum \mathbf{L} and spin angular momentum \mathbf{S} .

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

Recall that

$$\begin{aligned} L_x\psi &= -i\hbar \left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right) \psi & S_x\chi &= \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \chi \\ L_y\psi &= -i\hbar \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right) \psi & S_y\chi &= \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \chi \\ L_z\psi &= -i\hbar \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right) \psi & S_z\chi &= \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \chi \end{aligned}$$

Let Ψ be the product of wave function ψ and electron spinor χ .

$$\Psi = \psi\chi$$

Then

$$\mathbf{J}\Psi = \mathbf{L}\Psi + \mathbf{S}\Psi$$

Let J^2 be the magnitude-squared of total angular momentum.

$$J^2 = \mathbf{J} \cdot \mathbf{J} = J_x^2 + J_y^2 + J_z^2$$

Operator J^2 can be decomposed as

$$J^2 = (\mathbf{L} + \mathbf{S}) \cdot (\mathbf{L} + \mathbf{S}) = L^2 + S^2 + 2\mathbf{L} \cdot \mathbf{S}$$

In Eigenmath code

$$\mathbf{L} \cdot \mathbf{S}\Psi = \text{contract}(\mathbf{L}(\mathbf{S}(\Psi))) \quad (1)$$

The commutation relations for J^2 are

$$\begin{aligned} [J^2, L^2] &= 0 \\ [J^2, S^2] &= 0 \\ [J^2, J_x] &= 0 \\ [J^2, J_y] &= 0 \\ [J^2, J_z] &= 0 \\ [J^2, L_x] &= 2i\hbar(L_yS_z - L_zS_y) \\ [J^2, L_y] &= 2i\hbar(L_zS_x - L_xS_z) \\ [J^2, L_z] &= 2i\hbar(L_xS_y - L_yS_x) \\ [J^2, S_x] &= -2i\hbar(L_yS_z - L_zS_y) \\ [J^2, S_y] &= -2i\hbar(L_zS_x - L_xS_z) \\ [J^2, S_z] &= -2i\hbar(L_xS_y - L_yS_x) \end{aligned}$$