

## Block 7

### Step 2 - Time reversal and what it means for the molecule state (123 §60)

fundamental states in §60: the operation of time reversal on a spinor wave function  $\psi$  corresponds to taking the complex conjugate and applying a specific phase factor - for a spin-1/2 system,  $T: \psi \rightarrow i \sigma_y \psi^*$ .

The important consequence of this is that the spin operator  $\hat{S}$  changes sign under time reversal:  $T \hat{S} T^{-1} = -\hat{S}$ .

This means any state with  $\langle S \rangle \neq 0$  is not time-reversal symmetric, it distinguishes a preferred spin direction, which is exactly what time reversal would flip. For an isolated molecule in a singlet state, time reversal symmetry is preserved by construction: the two electrons pair with opposite spins and the net moment vanishes.  $\langle S_m \rangle = 0$  exactly.

When the molecule is coupled to the reservoir, the observables  $\langle S_{m \pm 2} \rangle$  become complex values, the reservoir introduces dissipation that breaks the constraint  $\langle S_{m+2} \rangle = \langle S_{m-2} \rangle^*$  that would otherwise force  $M_0$  to be real. Since  $M_0$  gets an imaginary part, the spectrum  $eg(\omega)$  shifts asymmetrically. A specific spin configuration is selected,  $\langle S_m \rangle \neq 0$ , and the system is ~~now~~ in a state that is not invariant under  $T$ . Time-reversal symmetry is spontaneously broken by the chirality and dissipative coupling to the reservoir.