Block II

The vibrational Hamiltonian and reservoir coupling

The vibrational part is

$$H_{vib} = \sum_i \omega_i b_i^\dagger b_i + \sum_{ijk} \Phi_{ijk} Q_i Q_j Q_k$$

describes harmonic molecular vibrations (first term) with anharmonic corrections (second term). The bosonic operators $b_i^\dagger$ and b_i create and destroy vibrational quanta. The displacement operator $Q_i = b_i + b_i^\dagger$ represents nuclear motion. The anharmonic term Φ_{ijk} is allowed by symmetry precisely because a chiral molecule has no inversion symmetry, odd-order terms are not forbidden.

The electrons and vibrations couple through $H_1, \sum_i Q_i$ inside H_{mol}: when an electron hops, it can simultaneously excite or absorb a molecular vibration. The coupling matrix H_1 carries the same geometric structure as H_0 but with amplitudes t_1 and λ_1 for the vibrationally-assisted processes.

The reservoir coupling:

$$H_T = \sum_{k\in L} \psi_k^\dagger U_{k1} \psi_1 + \sum_k$$ connects the molecular endpoints to electron reservoirs. Electrons in the left (right) reservoir tunnel into site 1 (M) with amplitude U_{k1} (U_{kM}). This is the standard open-system Hamiltonian. The reservoirs are modelled as ideal Fermi gases at chemical potentials μ_L and μ_R.