Scattering solution of interacting Hamiltonian for electronic control of molecular spin qubits

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We theoretically study how a scattered electron can entangle molecular spin qubits (MSQs). This requires solving the inelastic transport of a single electron through a scattering region described by a tight-binding interacting Hamiltonian. We accomplish this using a Green's function solution. We can model realistic physical implementations of MSQs by parameterizing the tight-binding Hamiltonian with first-principles descriptions of magnetic anisotropy and exchange interactions. We find that for two-MSQ systems with inversion symmetry, the spin degree of freedom of the scattered electron offers probabilistic control of the degree of entanglement between the MSQs.