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Quantum Molecular Magnetism SYLVAIN BRECHET, FRANCOIS REUSE, KLAUS MASCHKE, JEAN-PHILIPPE ANSERMET, EPFL — Our theoretical description of quantum molecular magnetism is based on the quantum master equations, where the system consists of the electronic spin degrees of freedom and the bath consists of the remaining degrees of freedom. The system is weakly coupled and weakly correlated to the bath, which is at equilibrium on an appropriate time scale. The electrons satisfy the exclusion principle, which requires the tensorial product of the spin and orbital parts of the state to be antisymmetric under permutation. However, the symmetries of the parts of the state taken separately are determined by the irreducible unitary representations of the permutation group. The structure of the quantum master equations is also determined by these representations. The coupling between different isotypic components of the permutation group appearing in the quantum master equations leads to a description of magnetic dissipation at the molecular level and defines molecular spin selection rules. Thus, this theoretical description is expected to bring new and fundamental insight for molecular magnetism. In particular, it is expected to predict the non-trivial deflection of molecular clusters in a field gradient.

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