# Spin-orbit coupling with the spin-adapted density matrix renormalization group

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We present a method to include the effects of spin-orbit coupling in density matrix renormalization group (DMRG) theory. In our approach both the wavefunctions of the interacting electronic states and their transition density matrices are obtained using a spin-adapted DMRG ansatz. The spin-orbit coupling operator is evaluated in a basis of correlated DMRG wave functions, using a mean-field approximation of the spin-orbit interaction. The proposed scheme was implemented within the BLOCK DMRG program. To demonstrate the power of this method, we have computed zero-field splittings (splitting of classically degenerate states due to the relativistic spin-orbit interaction) in transition metal atoms and molecules including up to 57 orbitals in the active space. These results show the method's potential for computing reliable and accurate spin-orbit coupled energies and SOC matrix elements.