P48 – Longitudinal static (hyper)polarizabilities of one-dimensional chemical systems, obtained with SU(2)xU(1) invariant matrix product states

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The density matrix renormalization group outperforms other high accuracy methods for one-dimensional systems. The reason is its underlying matrix product state (MPS) Ansatz, which efficiently captures the quantum entanglement properties of low-lying eigenstates. This allows to reach exact diagonalization accuracy within a reasonable amount of time. We have implemented a sweep algorithm for the variational optimization of SU(2)xU(1) (spin and particle number) invariant MPSs for general real-valued Hamiltonians. This class also includes non-relativistic quantum chemical systems within the Born-Oppenheimer approximation. We present finite field results of the longitudinal static polarizabilities and second hyperpolarizabilities of one-dimensional chemical chains.