Matrix product states and their uses in quantum chemistry

Sebastian Wouters[1,3], Peter A. Limacher[2], Dimitri Van Neck[1] and Paul W. Ayers[2]

[1] *Center for Molecular Modeling, Ghent University, Ghent, Belgium*
[2] *Department of Chemistry, McMaster University, Hamilton, Ontario, Canada*
[3] *sebastian.wouters@ugent.be*

ABSTRACT Renormalization group techniques have allowed to answer many questions in physics, ranging from phase transitions to the perceivable properties of quantum fields. Their main idea is to identify the important degrees of freedom of a problem and impose plausible assumptions on the others. In this talk one particular technique, the density matrix renormalization group, will be discussed. The techique works particularly well for one-dimensional systems. This can be explained by means of its underlying Ansatz, the matrix product state, and one of the central quantities from quantum information theory, quantum entanglement. But once an Ansatz is available, the technique can be used for any (also not one-dimensional) system. Convergence becomes harder in that case. We will give a brief general introduction to the subject.

We have implemented the single-site sweep algorithm for the variational optimization of SU(2) $\times$ U(1) (spin and particle number) invariant matrix product states for general spin and particle number symmetric fermionic Hamiltonians. This class also includes non-relativistic quantum chemical systems within the Born-Oppenheimer approximation. High-accuracy ab-initio finite field results of the longitudinal static polarizabilities and second hyperpolarizabilities of one-dimensional hydrogen chains are obtained with the algorithm. A comparison with other methods is made.

References:

[1] White, S. R. and Martin, R. L. *Journal of Chemical Physics*, 110 (1999) 4127-4130.

[2] Schollwöck, U. *Annals of Physics*, 326 (2011) 96-192.

[3] McCulloch, I. P. and Gulácsi, M. *Europhysics Letters*, 57 (2002) 852-858.

[4] Singh, S., Pfeifer, R. N. C. and Vidal, G. *Physical Review A*, 82 (2010) 050301.

[5] Champagne, B. and Kirtman, B. *International Journal of Quantum Chemistry*, 109 (2009) 3103-3111.

[6] Wouters, S., Limacher, P. A., Van Neck, D. and Ayers, P. W. *arXiv*:1111.5701v1 [cond-mat.str-el]