A Few Things I Learned About Tensor Product Methods in Quantum Chemistry

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1 Tensor product states

1.1 Intro

A quantum mechanical wavefunction can be represented as a tensor, T. Some quantum chemical methods, such as DMRG (Density Matrix Renormalization Group) theory approximates this tensor as a product of N order-2 and -3 tensors. Tensor product (TP) methods are very successful in describing structurally simple, strongly correlated systems.

1.2 Occuptation number representation

A tensor product state is most easily described using occupation number representation, in which a determinant is represented as a string of numbers indicating the occupancy of each orbital. In the spin-orbital formalism, where occupation numbers can be either 0 or 1, a ground-state configuration may be written

$$|1111000000\ldots\rangle \tag{1}$$

where the first four orbitals are occupied and the rest are unoccupied.

1.3 Tensor product states

A general Fock-space state written using the occupancy-number notation appears as:

$$|\psi_{\mathrm{TP}}\rangle = \sum_{n_1,n_2,\ldots,n_M} c_{n_1,n_2,\ldots,n_M} |n_1 n_2 \ldots n_M\rangle \tag{2}$$

Note that this is a general Fock-space state, as there is no restriction on the number of particles in any term. In TPS methods, the total wavefunction is represented as a tensor composed of these coefficients, setting equal to zero all coefficients corresponding to states with a number of electrons not consistent with the physical system being considered. In a system of M orbitals, there are 2^M such coefficients. In matrix product state (MPS) methods, this M-mode tensor is approximated as a network of M 2- and 3-order tensors:

$$\bar{C}_{n_1,n_2,\ldots,n_M} \approx \sum_{b_1,b_2\ldots b_{M-1}} w^1_{n_1,b_1} w^2_{b_1,n_2,b_2} \ldots w^{M-1}_{b_{M-2},n_{M-1},b_{M-1}} w^M_{b_{M-1},n_M} \tag{3}$$

where each w^i is an order-2 or order-3 tensor, and there are $M-1$ contractions over the set $\{\, b^i \,\}$ of internal indices. The decomposition is a purely mathematical approximation, and the resultant low-order tensors do not have an intuitive physical meaning, although the goal of the decomposition is naturally to minimize the lost entanglement or electronic structure information.

This notation allows for a compact representation of any arbitrary state in Fock space. The Density Matrix Renormalization Group (DMRG) algorithm, which variationally optimizes MPS tensors, is one of the most prominent tensor network methods in electronic structure theory.[1–3]

TP methods are very efficient in determining low-energy states of 1-D systems, but the rapidly increasing complexity of the tensor network representation for 3-D or otherwise complicated electronic states generally makes study of most 3-D systems intractable.[4] In spite of its efficiency, the computational complexity severely limits the possible applications. Extending TPS methods to higher-dimensional systems is an active area of research, and many of these methods can describe strongly correlated systems.[5–12]

2 Further reading and influences

If you'd like to know more about tensor product state methods, you can just get bent, because it no one seems to have written a comprehensible and comprehensive description of them; I read books and papers for a while, but ended up synsthesizing this from a mash-up of what I could understand and remember from the comments of 3 different people with Ph.D.s, all of whom, of course, gave very different descriptions.

References

(1) White, S. R. *Physical Review Letters* **1992**, *69*, 2863–2866.

(2) White, S. R. *Physical Review B* **1993**, *48*, 10345–10356.

(3) White, S. R.; Martin, R. L. *The Journal of Chemical Physics* **1999**, *110*, 4127–4130.

(4) Chan, G. K.-L.; Sharma, S. *Annual Review of Physical Chemistry* **2011**, *62*, 465–481.

(5) Jordan, J.; Orús, R.; Vidal, G.; Verstraete, F.; Cirac, J. I. *Physical Review Letters* **2008**, *101*, 250602.

(6) Kovyrshin, A.; Reiher, M. *The Journal of Chemical Physics* **2017**, *147*, 214111.

(7) Marti, K. H.; Bauer, B.; Reiher, M.; Troyer, M.; Verstraete, F. *New Journal of Physics* **2010**, *12*, 103008.

(8) Murg, V.; Verstraete, F.; Schneider, R.; Nagy, P. R.; Legeza, Ö. *Journal of Chemical Theory and Computation* **2015**, *11*, 1027–1036.

(9) Szalay, S.; Pfeffer, M.; Murg, V.; Barcza, G.; Verstraete, F.; Schneider, R.; Legeza, Ö. *International Journal of Quantum Chemistry* **2015**, *115*, 1342–1391.

(10) Nakatani, N.; Chan, G. K.-L. *The Journal of Chemical Physics* **2013**, *138*, 134113.

(11) Abraham, V.; Mayhall, N. J. *Journal of Chemical Theory and Computation* **2020**, *16*, 6098–6113.

(12) Abraham, V.; Mayhall, N. J. *The Journal of Chemical Physics* **2021**, *155*, 054101.