Recent theoretical results on the QC-DMRG method

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I will present some recent theoretical results on the QC-DMRG method, including

- the fact that with bond dimension 3 and optimized orbitals it is exact for two-electron wavefunctions [1]
- the exact formulation of the infinite basis limit by a half-infinite chain of MPS matrices of increasing size [2]
- a power law scaling of errors for the restricted active space density matrix renormalization group (DMRG-RAS) method [3].

These results are illustrated by numerical calculations for diatomic molecules and - in case of [3] - the FeMoco complex.

[1] G. F. Gergely Barcza, J. Math. Phys., **63** (2022), 091901.
[2] G. F. Gergely Barcza, Ö. Legeza, J. Chem. Phys., **105** (2022), 165144.
[3] G. F., Gergely Barcza, Ö. Legeza, arXiv:2111.06665.