At this point it is worthwhile mentioning that it has been proposed [100] that in the special case of compressing an MPO-MPS product, an important speedup over the standard methods may be achieved: SVD may be very slow if normalization has to be carried out first at a cost $O(D_W^3 D^3)$, but a good starting point for the variational method would be essential to have. But the proposed solution from SVD compression may not be bad if the block states are almost orthonormal and it seems that in the MPO-MPS product case this is essentially true if both the MPO and the MPS were in canonical form (for the MPO again formed by looking at the double index as one big index), which can be achieved at much lower cost ($O(dD^3)$ and $O(d^2 D_W^3)$, where $D_W \ll D$ usually, versus $O(dD^3 D_W^3)$). Even if the proposed compression is not too good, it will still present a much better starting point for the variational compression. So the procedure would be: (i) bring both MPO and MPS in the same canonical form; (ii) do SVD compression, of course only multiplying out MPO and MPS matrices on the fly; (iii) use this as variational input if you don't trust the result too much.

6. Ground state calculations with MPS

Assume we want to find the ground state of some Hamiltonian $\hat{H}$. In order to find the optimal approximation to it, we have to find the MPS $|\psi\rangle$ of some dimension D that minimizes

$$E = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{181}$$

The most efficient way of doing this (in particular compared to an imaginary time evolution starting from some random state, which is also possible) is a variational search in the MPS space. In order to make this algorithm transparent, let us first express $\hat{H}$ as an MPO.

6.1. MPO representation of Hamiltonians

Due to the product structure inherent in the MPO representation, it might seem a hopeless task – despite its guaranteed existence – to explicitly construct a compact MPO representation for a Hamiltonian such as

$$\hat{H} = \sum_{i=1}^{L-1} \frac{J}{2}\hat{S}^+_i \hat{S}^-_{i+1} + \frac{J}{2}\hat{S}^-_i \hat{S}^+_{i+1} + J^z \hat{S}^z_i \hat{S}^z_{i+1} - h \sum_i \hat{S}^z_i. \tag{182}$$

This common notation is of course an abbreviation for sums of tensor products of operators:

$$\begin{aligned}\hat{H} \quad = \quad & J^z \hat{S}^z_1 \otimes \hat{S}^z_2 \otimes \hat{I} \otimes \hat{I} \otimes \hat{I} \ldots + \\ & \hat{I} \otimes J^z \hat{S}^z_2 \otimes \hat{S}^z_3 \otimes \hat{I} \otimes \hat{I} \ldots + \\ & \ldots\end{aligned}$$

It is however surprisingly easy to express this sum of tensor products in MPO form [70] – to this purpose it is convenient to reconsider the building block $W^{\sigma\sigma'}_{bb'}$ combined with its associated projector $|\sigma\rangle\langle\sigma'|$ to become an operator-valued matrix $\hat{W}_{bb'} = \sum_{\sigma\sigma'} W^{\sigma\sigma'}_{bb'} |\sigma\rangle\langle\sigma'|$ such that the MPO takes the simple form

$$\hat{O} = \hat{W}^{[1]} \hat{W}^{[2]} \ldots \hat{W}^{[L]}. \tag{183}$$

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Each $\hat{W}^{[i]}$ acts on a different local Hilbert space at site i, whose tensor product gives the global Hilbert space. Multiplying such operator-valued matrices yields sums of tensor products of operators such that expressing $\hat{H}$ in a compact form seems feasible.

To understand the construction, we move through an arbitrary operator string appearing in $\hat{H}$: starting from the right end, the string contains unit operators, until at one point we encounter one of (in our example) 4 non-trivial operators. For the field operator, the string part further to the left may only contain unit operators; for the interaction operators, the complementary operator must follow immediately to complete the interaction term, to be continued by unit operators further to the left. For book-keeping, we introduce 5 corresponding states of the string at some given bond: state 1: only units to the right, states 2,3,4: one $\hat{S}^+$, $\hat{S}^-$, $\hat{S}^z$ just to the right, state 5: completed interaction or field term $-h\hat{S}^z$ somewhere to the right. Comparing the state of a string left and right of one site, only a few transitions are allowed: $1 \to 1$ by the unit operator $\hat{I}$, $1 \to 2$ by $\hat{S}^+$, $1 \to 3$ by $\hat{S}^-$, $1 \to 4$ by $\hat{S}^z$, $1 \to 5$ by $-h\hat{S}^z$. Furthermore $2 \to 5$ by $(J/2)\hat{S}^-$, $3 \to 5$ by $(J/2)\hat{S}^+$ and $4 \to 5$ by $J^z\hat{S}^z$, to complete the interaction term, and $5 \to 5$ for a completed interaction by the unit operator $\hat{I}$. Furthermore all string states must start at 1 to the right of the last site and end at 5 (i.e. the dimension D_W of the MPO to be) to the left of the first site. This can now be encoded by the following operator-valued matrices:

$$\hat{W}^{[i]} = \begin{bmatrix} \hat{I} & 0 & 0 & 0 & 0 \\ \hat{S}^+ & 0 & 0 & 0 & 0 \\ \hat{S}^- & 0 & 0 & 0 & 0 \\ \hat{S}^z & 0 & 0 & 0 & 0 \\ -h\hat{S}^z & (J/2)\hat{S}^- & (J/2)\hat{S}^+ & J^z\hat{S}^z & \hat{I} \end{bmatrix} \tag{184}$$

and on the first and last sites

$$\hat{W}^{[1]} = \begin{bmatrix} -h\hat{S}^z & (J/2)\hat{S}^- & (J/2)\hat{S}^+ & J^z\hat{S}^z & \hat{I} \end{bmatrix} \qquad \hat{W}^{[L]} = \begin{bmatrix} \hat{I} \\ \hat{S}^+ \\ \hat{S}^- \\ \hat{S}^z \\ -h\hat{S}^z \end{bmatrix}. \tag{185}$$

Indeed, a simple multiplication shows how the Hamiltonian emerges. Inserting the explicit operator representations gives the desired $W^{\sigma\sigma'}$-matrices for the MPO. It is therefore possible to express Hamiltonians exactly in a very compact MPO form; a similar set of rules leading to the same result has been given by [101].

For longer-ranged Hamiltonians, further "intermediate states" have to be introduced. Let us consider a model with just $\hat{S}^z\hat{S}^z$-interactions, but between nearest and next-nearest neighbours,

$$\hat{H} = J_1 \sum_i \hat{S}^z_i \hat{S}^z_{i+1} + J_2 \sum_i \hat{S}^z_i \hat{S}^z_{i+2}. \tag{186}$$

Then the bulk operator would read

$$\hat{W}^{[i]} = \begin{bmatrix} \hat{I} & 0 & 0 & 0 \\ \hat{S}^z & 0 & 0 & 0 \\ 0 & \hat{I} & 0 & 0 \\ 0 & J_1\hat{S}^z & J_2\hat{S}^z & \hat{I} \end{bmatrix}. \tag{187}$$

While the J_1-interaction can be encoded as before (moving as $1 \to 2 \to 4$), for the next-nearest neighbour interaction, one has to insert an additional step between 2 and 4, an intermediate state 3, where exactly one identity is inserted (moving as $1 \to 2 \to 3 \to 4$). It merely serves as a book-keeping device. Similarly, one can construct longer-ranged interactions. Except the top-left and botton-right corner, the non-vanishing parts of $\hat{W}^{[i]}$ are all below the diagonal by construction.

It might seem that for longer-ranged interactions the dimension D_W will grow rapidly as more and more intermediate states are needed (one additional state per unit of interaction range and per interaction term). While this is true in general, important exceptions are known which can be formulated much more compactly [74, 101]; consider for example the following exponentially decaying interaction strength $J(r) = Je^{-r/\xi} = J\lambda^r$, where $r > 0$ and $\lambda = \exp(-1/\xi)$. An interaction term $\sum_r J(r)\hat{S}^z_i\hat{S}^z_{i+r}$ would be captured by a bulk operator

$$\hat{W}^{[i]} = \begin{bmatrix} \hat{I} & 0 & 0 \\ \hat{S}^z & \lambda\hat{I} & 0 \\ 0 & J\lambda\hat{S}^z & \hat{I} \end{bmatrix}. \tag{188}$$

But even if such a simplification does not occur, it turns out that MPOs with quite small dimensions and moderate loss of accuracy can be found, either by approximating an arbitrary interaction function $J(r)$ by a sum of exponentials coded as above[72, 101], minimizing the L_2 distance $\|J(r) - \sum_{i=1}^n \alpha_i\lambda_i^r\|$ in α_i, λ_i, where n is given by the D_W and loss of accuracy one is willing to consider. Alternatively [74], one can of course construct the exact MPO where feasible and compress it by adapting MPS compression techniques to an acceptable D_W (and loss of accuracy).

6.2. Applying a Hamiltonian MPO to a mixed canonical state

Let us consider $|\psi\rangle$ in the following mixed canonical representation, identical to the single-site DMRG representation,

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} A^{\sigma_1}\dots A^{\sigma_{\ell-1}}\Psi^{\sigma_\ell}B^{\sigma_{\ell+1}}\dots B^{\sigma_L}|\boldsymbol{\sigma}\rangle \tag{189}$$

or

$$|\psi\rangle = \sum_{a_{\ell-1},a_\ell} |a_{\ell-1}\rangle_A \Psi^{\sigma_\ell}_{a_{\ell-1},a_\ell}|a_\ell\rangle_B. \tag{190}$$

Let us now look at the matrix elements $\langle a_{\ell-1}\sigma_\ell a_\ell|\hat{H}|a'_{\ell-1}\sigma'_\ell a'_\ell\rangle$ obtained using the MPO representation for $\hat{H}$. By inserting twice the identity $\hat{I} = \sum_{\boldsymbol{\sigma}} |\boldsymbol{\sigma}\rangle\langle\boldsymbol{\sigma}|$, we obtain (the sums with a star exclude site ℓ)

$$\begin{aligned}
& \langle a_{\ell-1}\sigma_\ell a_\ell|\hat{H}|a'_{\ell-1}\sigma'_\ell a'_\ell\rangle \\
= & \sum_{\boldsymbol{\sigma}}\sum_{\boldsymbol{\sigma}'} W^{\sigma_1,\sigma'_1}\dots W^{\sigma_L,\sigma'_L}\langle a_{\ell-1}\sigma_\ell a_\ell|\boldsymbol{\sigma}\rangle\langle\boldsymbol{\sigma}'|a'_{\ell-1}\sigma'_\ell a'_\ell\rangle \\
= & \sum_{\boldsymbol{\sigma}*}\sum_{\boldsymbol{\sigma}'*} W^{\sigma_1,\sigma'_1}\dots W^{\sigma_\ell,\sigma'_\ell}\dots W^{\sigma_L,\sigma'_L} \\
& \langle a_{\ell-1}|\sigma_1\dots\sigma_{\ell-1}\rangle\langle a_\ell|\sigma_{\ell+1}\dots\sigma_L\rangle\langle\sigma'_1\dots\sigma'_{\ell-1}|a'_{\ell-1}\rangle\langle\sigma'_{\ell+1}\dots\sigma'_L|a'_\ell\rangle \\
= & \sum_{\boldsymbol{\sigma}*}\sum_{\boldsymbol{\sigma}'*} W^{\sigma_1,\sigma'_1}\dots W^{\sigma_\ell,\sigma'_\ell}\dots W^{\sigma_L,\sigma'_L}
\end{aligned}$$