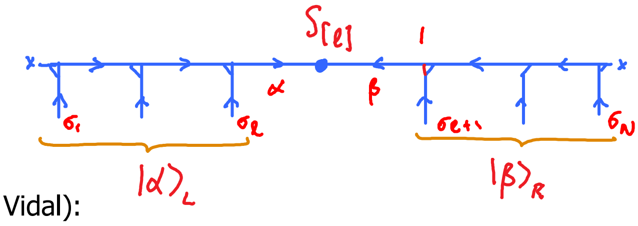
## MPS VI: Gamma-Lambda Notation

[Vidal2003], [Schollwöck2011, Sec. 4.6]



Usual bond-canonical form of MPS:

$$|\psi\rangle = |\beta\rangle_{\ell,R}\,|\alpha\rangle_{\ell,L}\,S^{\alpha\beta}_{[\ell]} \qquad (1)$$




Choose $S$ diagonal, and call it $\Lambda$ (following Vidal):

$$|\psi\rangle = |\alpha\rangle_{\ell,R}\,|\alpha\rangle_{\ell,L}\,\Lambda^{\alpha\alpha}_{[\ell]} \qquad (2)$$

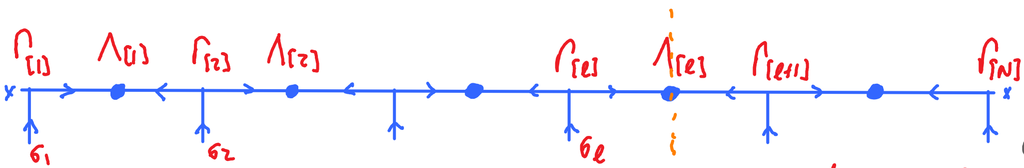
Then reduced density matrices of left and right parts are diagonal, with eigenvalues $\left(\Lambda^{\alpha\alpha}_{[\ell]}\right)^2$ :

$$\rho_L = \mathrm{Tr}_R\,|\psi\rangle\langle\psi| = \sum_\alpha |\alpha\rangle_{\ell,L}\,\underbrace{\left(\Lambda^{\alpha\alpha}_{[\ell]}\right)^2}_{\rho^{\alpha\alpha}_{[\ell]L}}\,{}_{\ell,L}\langle\alpha| \qquad (3)$$

$$\rho_R = \mathrm{Tr}_L\,|\psi\rangle\langle\psi| = \sum_\alpha |\alpha\rangle_{\ell,R}\,\underbrace{\left(\Lambda^{\alpha\alpha}_{[\ell]}\right)^2}_{\rho^{\alpha\alpha}_{[\ell]R}}\,{}_{\ell,R}\langle\alpha| \qquad (4)$$

Vidal introduced MPS representation in which Schmidt decomposition can be read off for each bond:

$$|\psi\rangle = \qquad (5)$$




between site $\ell$, $\ell+1$

where $\Lambda_{[\ell]}$ = diagonal matrix, consisting of Schmidt coefficients w.r.t. to bond $\ell$ , i.e.

$$|\psi\rangle = |\alpha\rangle_{\ell,R}\,|\alpha\rangle_{\ell,L}\,\Lambda^{\alpha\alpha}_{[\ell]}\,, \qquad \rho_{[\ell]L} = \rho_{[\ell]R} = \Lambda^2_{[\ell]} \qquad (6)$$

with orthonormal sets on L:

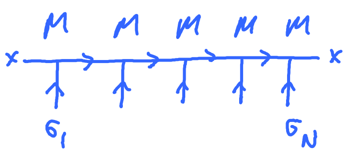
$$ {}_{\ell,L}\langle\alpha'|\alpha\rangle_{\ell,L} = \delta^{\alpha'}{}_{\alpha} \qquad (7)$$

and on R:

$$ {}_{\ell,R}\langle\alpha'|\alpha\rangle_{\ell,R} = \delta^{\alpha'}{}_{\alpha} \qquad (8)$$

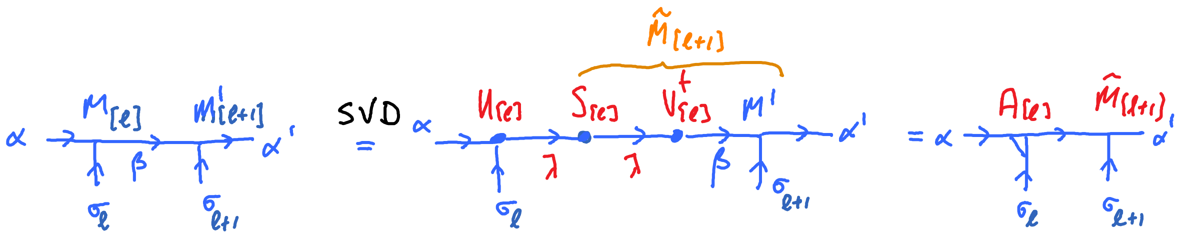
Any MPS can always be brought into $\Gamma\Lambda$ form. Proceed a same manner as when left-normalizing,
[cf. MPS-I.2]

$$|\psi\rangle = |\vec{\sigma}\rangle_N\left(M^{\sigma_1}\dots M^{\sigma_N}\right) \qquad (9)$$




Successively use SVD on pairs of adjacent tensors:

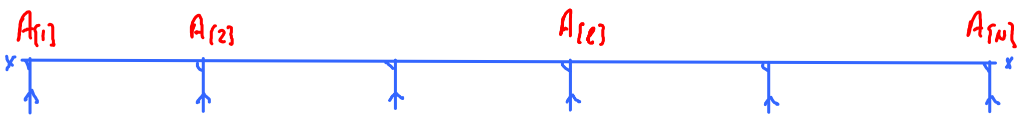
$$MM' = USV^\dagger M' \equiv A\tilde{M}\,, \qquad A = U\,, \quad \tilde{M} = SV^\dagger M' \qquad (10)$$




(11)

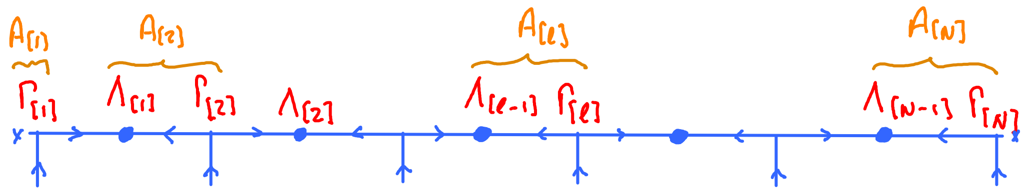
store singular values, $\Lambda_{[\ell]} = S_{[\ell]}$ and at end define $\Gamma^{\sigma_1}_{[1]} \equiv A^{\sigma_1}_{[1]}$, $\Lambda_{[\ell-1]}\Gamma^{\sigma_\ell}_{[\ell]} \equiv A^{\sigma_\ell}_{[\ell]}$. (12)

$|\psi\rangle =$




(13)

$\equiv$




(14)

Note: in numerical practice, this involves dividing by singular values, $\Gamma^{\sigma_\ell}_{[\ell]} \equiv \Lambda^{-1}_{[\ell-1]} A^{\sigma_\ell}_{[\ell]}$ (15)

So, first truncate states for which $S^{\alpha\alpha}_{[\ell-1]} = 0$, (16)

Even then, the procedure can be numerically unstable, since arbitrarily small singular values may arise.

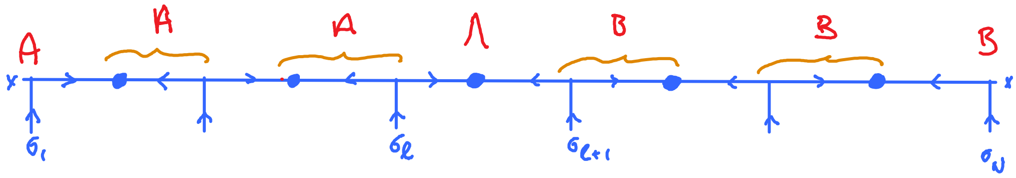
So, truncate states for which (say) $S^{\alpha\alpha}_{[\ell-1]} < 10^{-8}$. (17)

Similarly, if we start from the right, SVDs yield right-normalized $B$-tensors, and we can define

$$\Gamma^{\sigma_\ell}_{[\ell]} \Lambda_{[\ell]} \equiv B^{\sigma_\ell}_{[\ell]} \qquad (18)$$

So, relation between standard bond-canonical form and 'canonical $\Gamma\Lambda$ form' is:

$|\psi\rangle =$




(19)

$$\mathbb{1} = A^\dagger_{[\ell]\sigma} A^\sigma_{[\ell]} = \Gamma^\dagger_{[\ell]\sigma} \Lambda^\dagger_{[\ell-1]} \Lambda_{[\ell-1]} \Gamma^\sigma_{[\ell]} = \Gamma^\dagger_{[\ell]\sigma} \rho_{[\ell-1]R} \Gamma^\sigma_{[\ell]}$$

$$\mathbb{1} = B^\dagger_{[\ell]\sigma} B^\sigma_{[\ell]} = \Gamma^\dagger_{[\ell]\sigma} \Lambda^\dagger_{[\ell]} \Lambda_{[\ell]} \Gamma^\sigma_{[\ell]} = \Gamma^\dagger_{[\ell]\sigma} \rho_{[\ell]L} \Gamma^\sigma_{[\ell]}$$