Matrix Product Renormalization Group method

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Outline

- Introduction to automatic differentiation (AD)
- 1D implementation (essentially same as cMPO methods)
- 2D implementation
- Summary

Dual numbers

- A dual number is $a + b\varepsilon$ with a condition $\varepsilon^2 = 0$.
- Simply, ε can be regarded as an infinitesimal number.
  - Various functions/operations can be extended to dual numbers.
  - For example, $f(a + b\varepsilon) = f(a) + bf'(a)\varepsilon$.
- Mathematically this is a commutative ring $\mathbb{C}[\varepsilon]/\varepsilon^2$. This construction is nothing but an algebraic definition of a tangent space.

Forward-mode automatic differentiation

- The relation $f(a + b\varepsilon) = f(a) + bf'(a)\varepsilon$ can be used inversely to recover the derivative. This is called forward-mode automatic differentiation (AD).
- This is useful when f is a complicated composite function.
- In other words, the automatic differentiation “automatically” decomposes the derivative of composite functions based on the “chain rule” and gives you a correct answer (derivative).
  - cf. Usually, the so-called reverse-mode AD is more efficient.

Hyper-dual numbers

- A hyper-dual number is $a + b\varepsilon_1 + c\varepsilon_2 + d\varepsilon_1\varepsilon_2$ with conditions $\varepsilon_1^2 = 0$, $\varepsilon_2^2 = 0$, and $\varepsilon_1\varepsilon_2 = \varepsilon_2\varepsilon_1$.
- By hyper-dual numbers we can compute the derivative up to the second order in a similar way as in dual numbers.
  - cf. If we impose an anticommutation relation $\xi_1\xi_2 = -\xi_2\xi_1$, then it is a well-known Grassmann number, which is maybe useful to solve fermionic models like the Hubbard model (my speculation).

Trotter error zero limit

- Using this, we can directly take a Trotter error zero limit.
- $\Delta\tau = \varepsilon_1\varepsilon_2,\ \sqrt{\Delta\tau} = \dfrac{\varepsilon_1 + \varepsilon_2}{\sqrt{2}}$

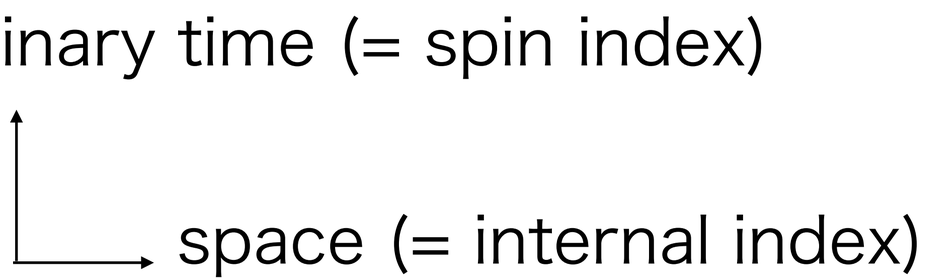
$$Z = \mathrm{tr}\, e^{-\beta H} = \mathrm{tr}\,(e^{-\Delta\tau H})^{\beta/\Delta\tau}$$

- Mathematically incorrect explanation:
  - If we put $\Delta\tau = 1/n$, then $Z = \mathrm{tr}\left(1 - \dfrac{H}{n}\right)^{\beta n} \to \mathrm{tr}\, e^{-\beta H} \quad (n \to \infty)$.
- I am not sure how to make this rigorous. I need help from mathematicians!

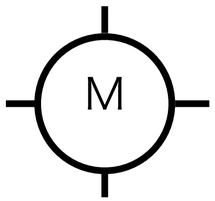
Hyper-dual number tensor networks

cMPO = continuous MPO

- $$H = -\sum_{j=1}^{N} (JS_j^z S_{j+1}^z + \Gamma S_j^x)$$



- Corresponding cMPO:



$$= \begin{pmatrix} 1 + \Gamma\varepsilon_1\varepsilon_2 S^x & \sqrt{J/2}(\varepsilon_1 + \varepsilon_2)S^z \\ \sqrt{J/2}(\varepsilon_1 + \varepsilon_2)S^z & 0 \end{pmatrix}$$

*S^x, S^z acting on the up-down indices

- Local many-body problems = contraction of (hyper- or hyper-hyper- or hyper-hyper-hyper-)dual number tensor networks.

1D implementation of MPRG

cMPS algorithm for 1D finite temperature

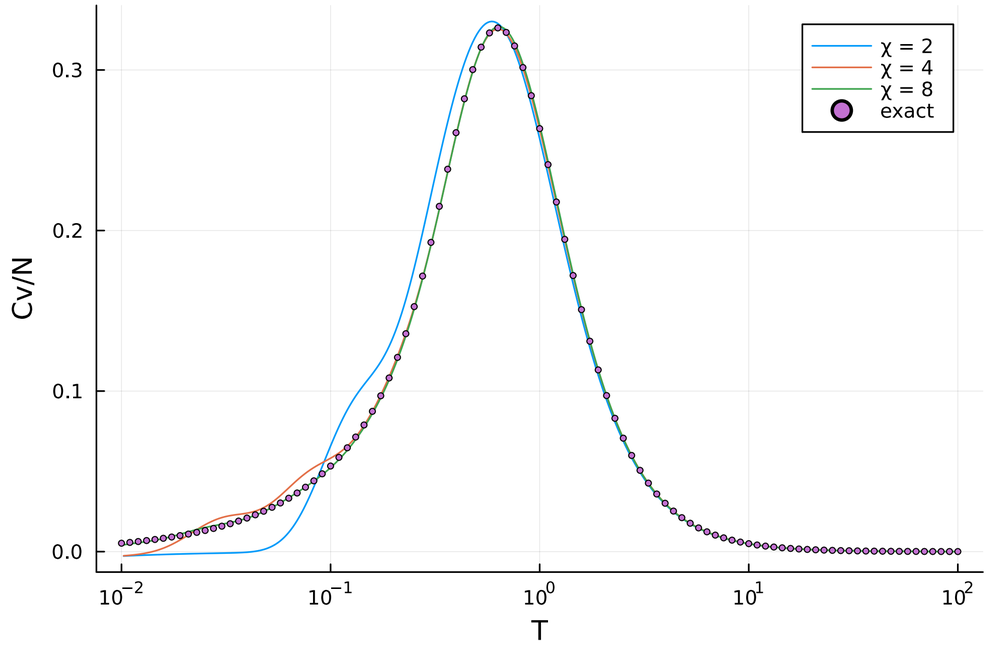
- As already explained, a 1D finite-temperature problem is reduced to finding a fixed point for some cMPO.
  - We can go to the finite temperature by (in some sense) imposing the periodic boundary condition. I will explain “in what sense” later.
- Of course, we can approximate the “eigenvector” by cMPS.
- Numerically, we use a finite bond dimension (χ) for cMPS and find the best solution for the fixed point iteration.

Essentially same idea (original of cMPO): Tang-Tu-Wang PRL **125**, 170604 (2020).

Example: 1D specific heat

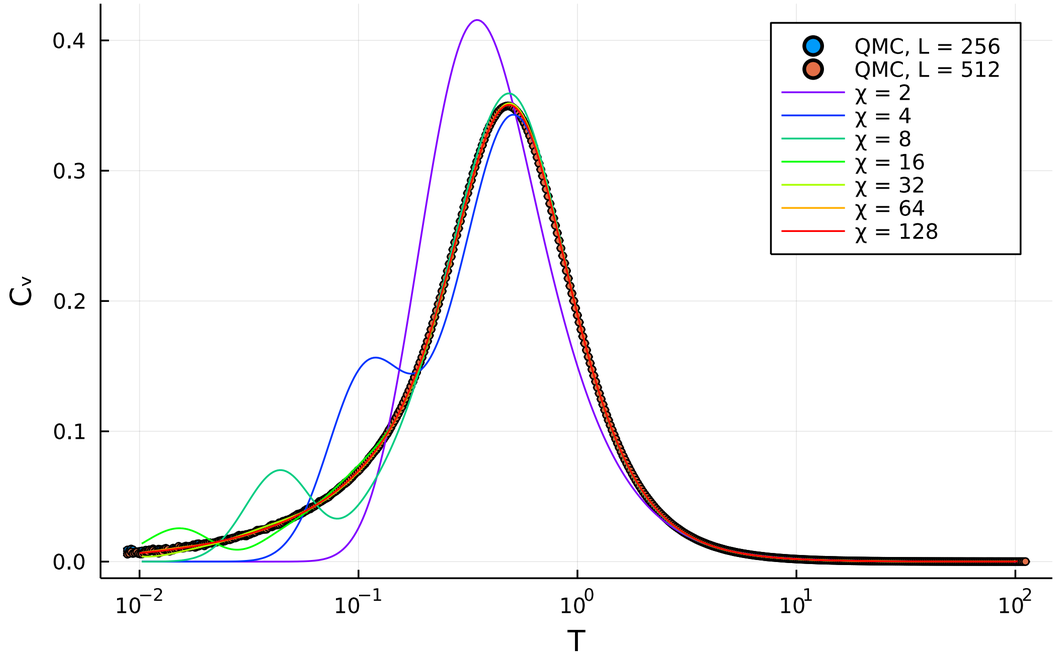
- Here's the benchmark for the cMPS & cMPS/MPS correspondence:

1D transverse field Ising model at criticality



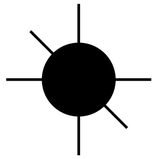
spin-1/2

AFM Heisenberg chain

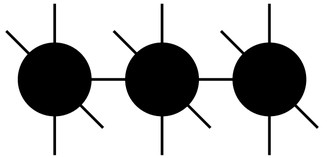


From cMPS to cPEPS

- The extension to 2D or 3D is direct in the MPRG formalism. This is the most important advantage of our method.

cPEPO: 

- 2D Hamiltonian -> rank-6 hyper-dual number tensor (cPEPO) -> diagonalization by cPEPS -> physical quantities.

cPEPS-> 

- This is simple, but technically still difficult. Currently we do not have a direct way of optimization, and we rather use a variational method.

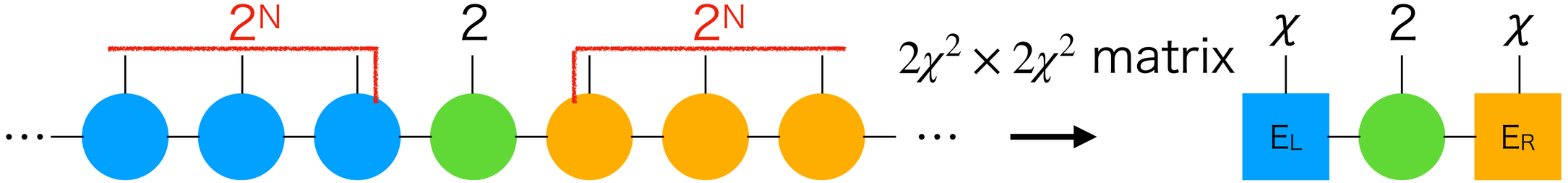
Going to 2D (quick demos)
Variational formulation of RG

“Pre-matrix product state” state

- White’s idea in 1992 is understandable as a “renormalization” of the “dimensional reduction” (DR).

Solving 1d many-body systems ≒ Variational optimization of 0d systems

  - Focusing on a single site (or two sites), place environments E_L & E_R.

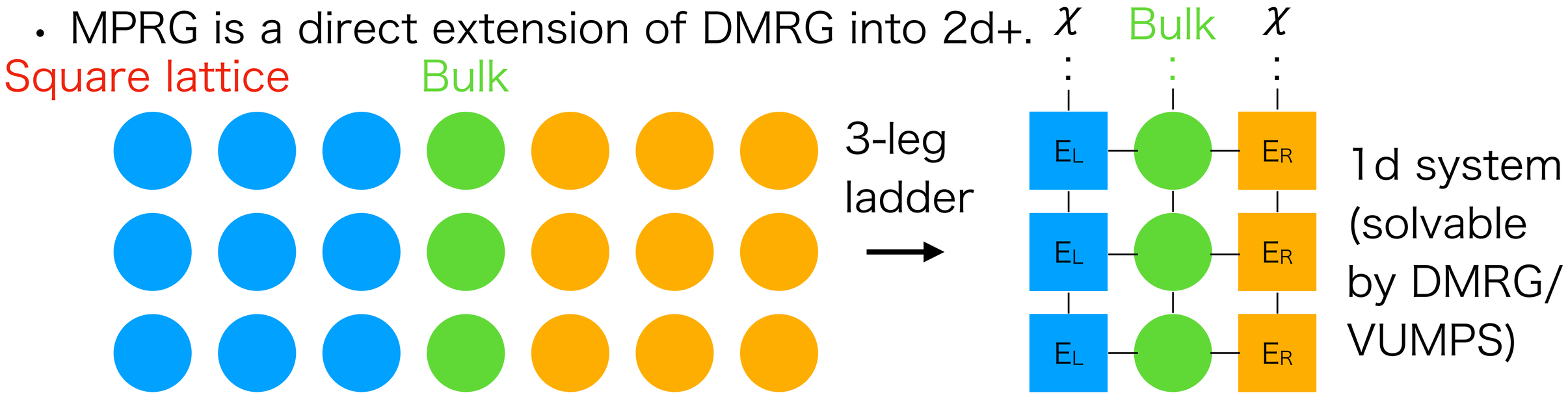


1d quantum system　　0d system (3 or 4 sites)

- Finally, the “DMRG sweep” solves it by renormalizing whole information into environments! This is an original idea of DMRG by White (1992).

MPRG is a higher-dimensional DMRG

- MPRG is a direct extension of DMRG into 2d+.



- The left boundary of Bulk is a left env., the right bdry. is a right env.

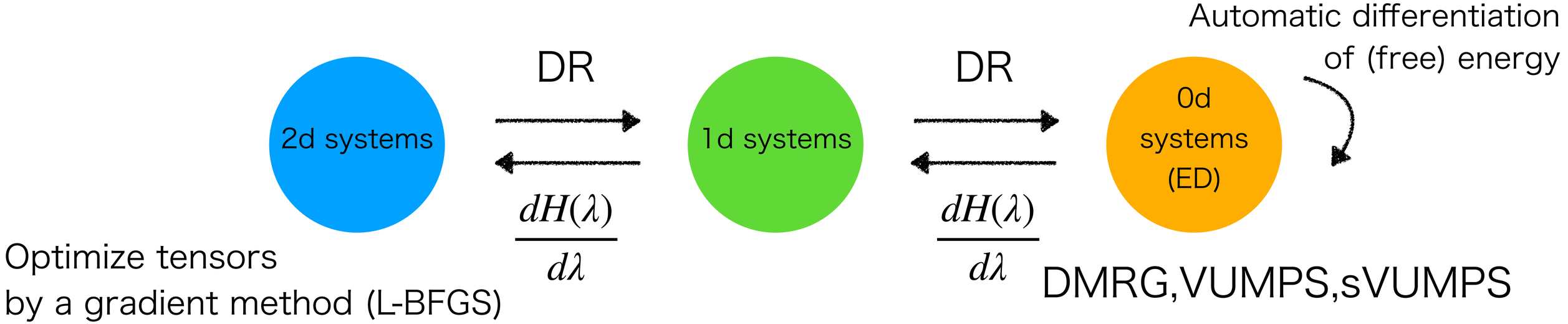
In any dimensions, it is ok if the “environments” finally reproduces the correct transfer matrix!

- Problem: is it possible to optimize E_L/E_R variationally by iterative DR?

Recursive Hellmann-Feynman theorem
- Poor man's way

- $\frac{dE(\lambda)}{d\lambda} = \langle\psi_\lambda|\frac{dH(\lambda)}{d\lambda}|\psi_\lambda\rangle$: HF theorem (Eigenpair property)

- Higher-dimensional Hermitian MPRG is done variationally by iterative Hellmann-Feynman thms. ← Chain rule application (Backpropagation)



MPRG

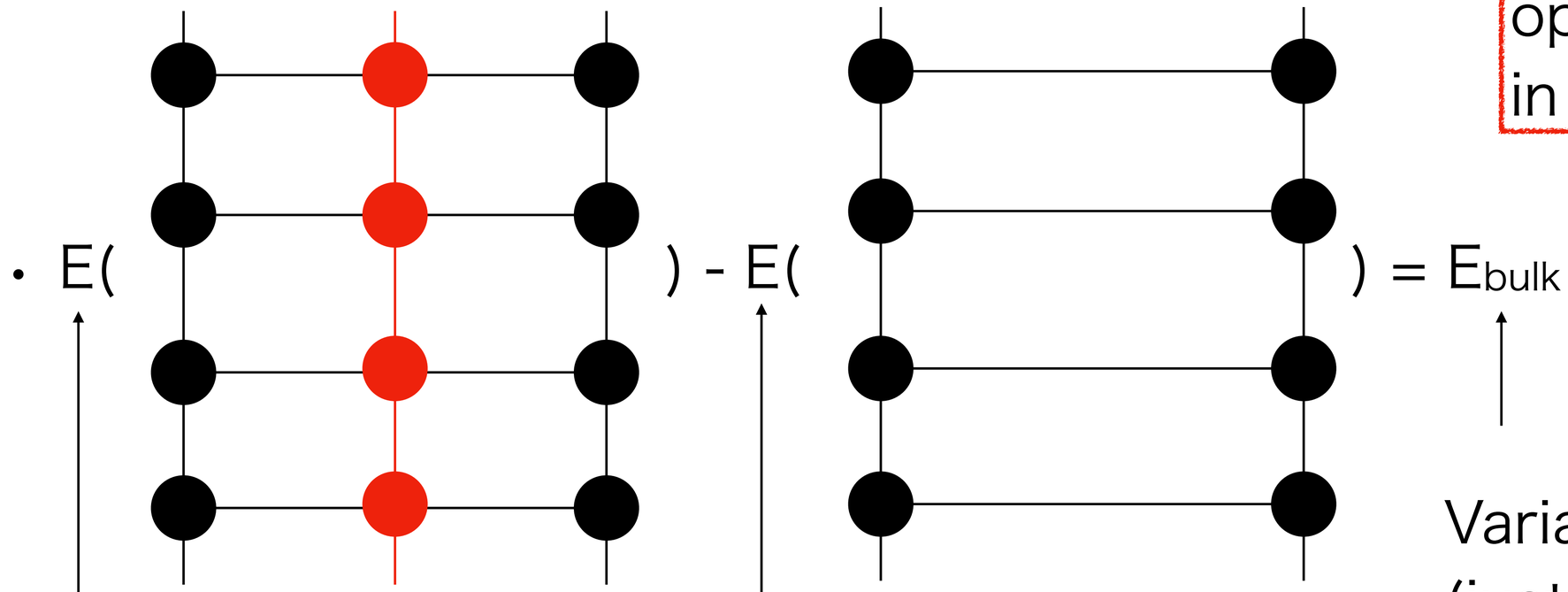
- Mathematically speaking,
  - 1d many-body problem → constrained variational optimization (on Riemannian mfd.)
  - 2d many-body problem → bilevel constrained variational optimization
  - 3d many-body problem → trilevel constrained variational optimization
- Finally, it gets a variational problem, but the essential idea is same as DMRG, i.e. “renormalization group” (iterative optimization of environments).

More details

3-leg ladder Hamiltonian

2-leg ladder Hamiltonian

This is very much similar to geometric optimization process in MD/DFT.



Variational optimization!
(just L-BFGS)

Roughly speaking,

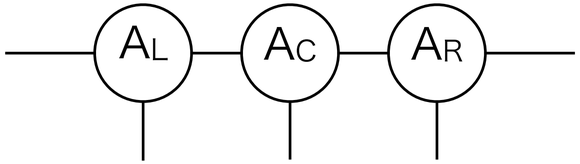
- Construct 3-leg/2-leg ladder Hamiltonians out of an arbitrary boundary interactions & optimization about boundary interactions.
- Very surprisingly, “(boundary + bulk) - boundary” contribution gives a good approximation of a correct 2D bulk system!
  - It seems like a very stupid idea,,, but it works!
- Roughly speaking, “optimized” boundary interactions behave as the correct (renormalized!) environment of the half-infinite space.

The MPRG!

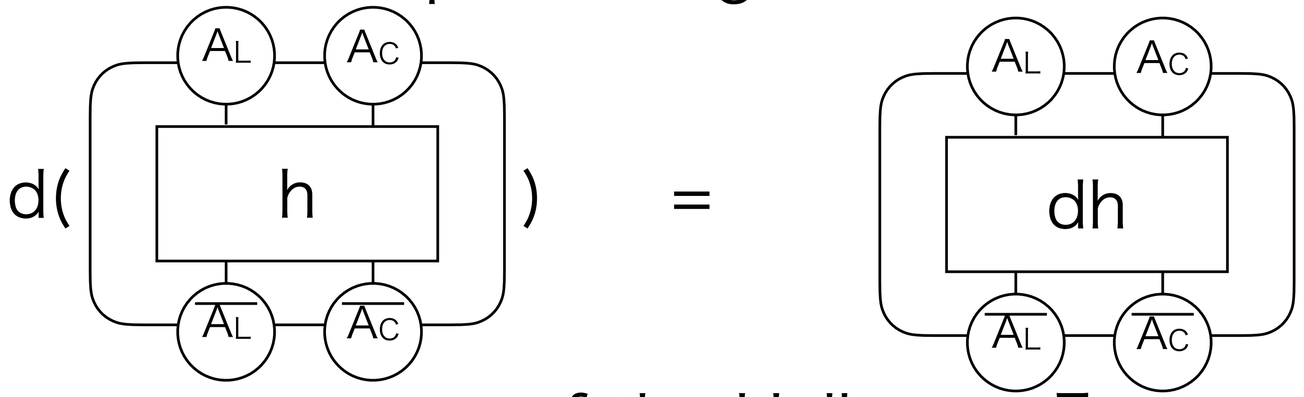
*In terms of MD/DFT, the boundary feels “the Hellmann-Feynman force”.

How can we do gradient optimization?

mixed canonical form:



- Q: How can we compute the gradient of E_{bulk}?



- This is a consequence of the Hellmann-Feynman theorem, but this gradient works even if the eigenvector is approximate, as first pointed out by B. Vanhecke *et al.* (e.g. in the YouTube video).

https://www.youtube.com/watch?v=efE0EekLcz4

[comment] VUMPS is a penalty method

- Regarding constrained optimization, VUMPS is a variant of a penalty method that is inefficient for our purpose.
- SuperVUMPS overcomes all the issues arising, i.e., using a complete Riemannian optimization to impose a constraint on manifolds.
  - Details are omitted today, but no local minimum problems were found in SuperVUMPS.

Check: https://github.com/MGYamada/SuperVUMPS.jl

- The original VUMPS is known to suffer from some issues.

M. Hauru *et al.*, SciPost Phys. **10**, 040 (2021).

Some results

- Ground state energy of the 2D Heisenberg model on the square lattice.

- I'd rather use (χ_1, χ_2) than a usual (χ, D).

- χ_1 is for MPS, and χ_2 is for (b/c)PEPS.

χ_2	PEPS	MPRG χ_1=8	MPRG χ_1=16
2	-0.66023	-0.66721	-0.66821
3*	-0.66788	-0.6676…	-0.66826

QMC: E = -0.6694

Summary

- We present 1D cMPS/cMPO/MPRG, and then 2D MPRG based on 1D techniques.
- Stability of the variational optimization allows us to correctly handle the quantum many-body problems.
- A lot of things are not done. We need more and more simulations.
  - Note: Today we only talk about the variational formulation of MPRG (vMPRG), but generally we can think of a power method version (power MPRG = pMPRG).