Introduction to Tensor Networks
Part 2

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Overview

The MPS manifold and its tangent space

Variational optimization

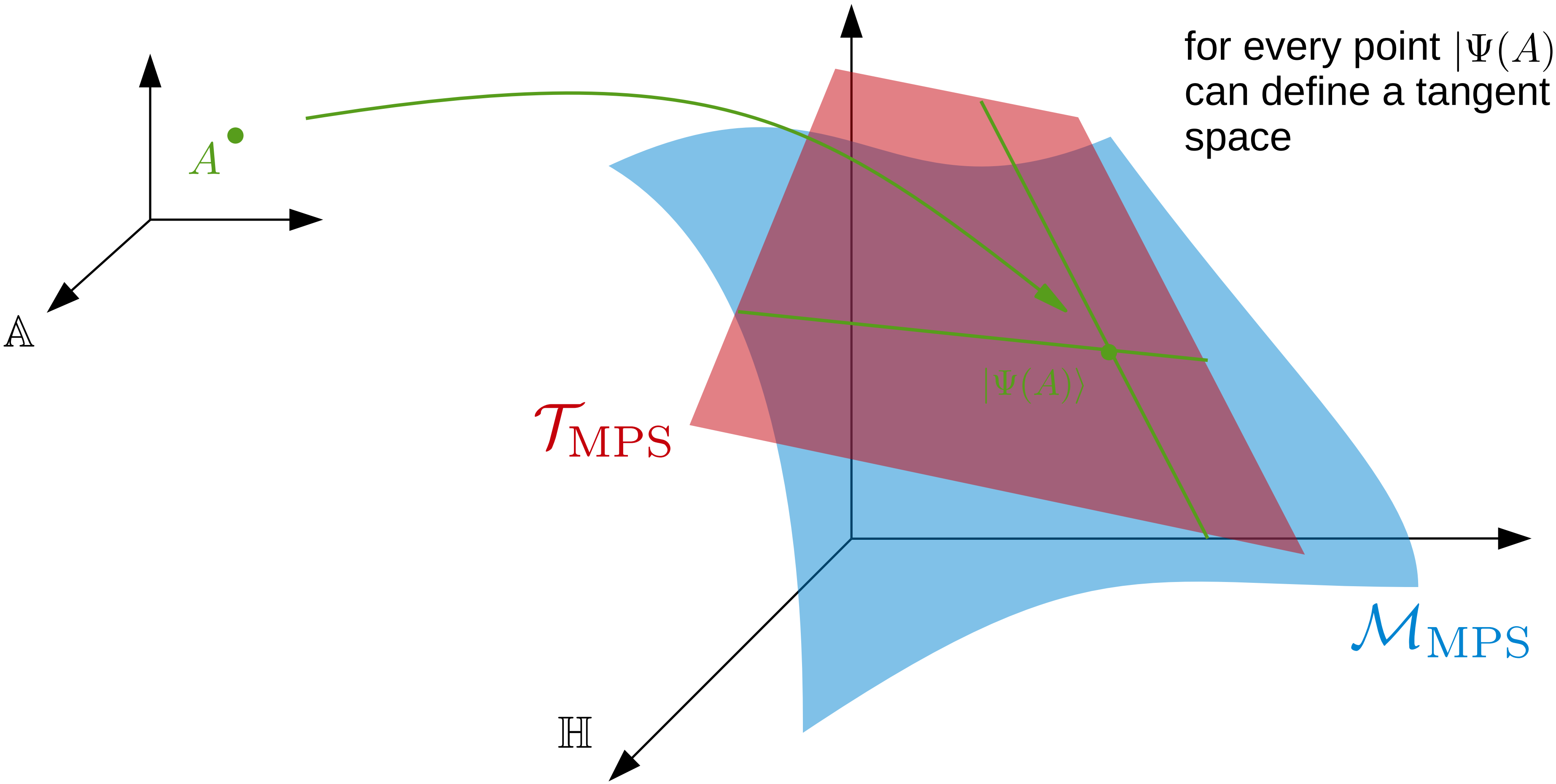
Time-dependent variational principle

Quasiparticle excitations

Outlook: PEPS

The MPS manifold and its tangent space

MPS/PEPS constitute a (non-linear) variational manifold $\mathcal{M}_{\mathrm{MPS}}$

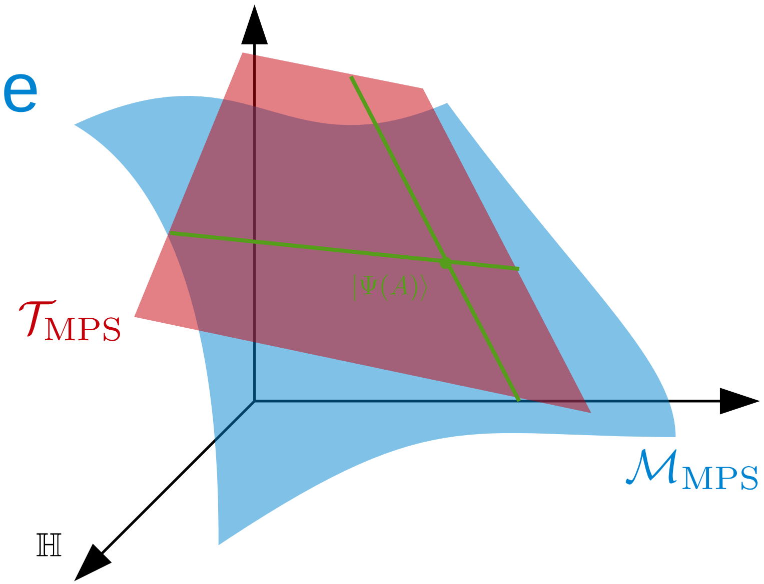


for every point $|\Psi(A)\rangle$, we can define a tangent space

The MPS manifold and its tangent space

$$|\Phi(B;A)\rangle = \sum_i B_i \frac{\partial}{\partial A_i} |\Psi(A)\rangle$$

$$= \sum_n \ldots - \underset{\ldots}{\boxed{A}} - \underset{s_{n-1}}{\boxed{A}} - \underset{s_n}{\boxed{B}} - \underset{s_{n+1}}{\boxed{A}} - \underset{\ldots}{\boxed{A}} - \ldots .$$



We can interpret a tangent vector as a local perturbation on a strongly-correlated background state

this perturbation is non-extensive

carries the notion of a quasiparticle

tangent space parametrizes the low-energy subspace on a given reference state

General idea: In order to capture low-energy dynamics, we have to leave the MPS/PEPS manifold

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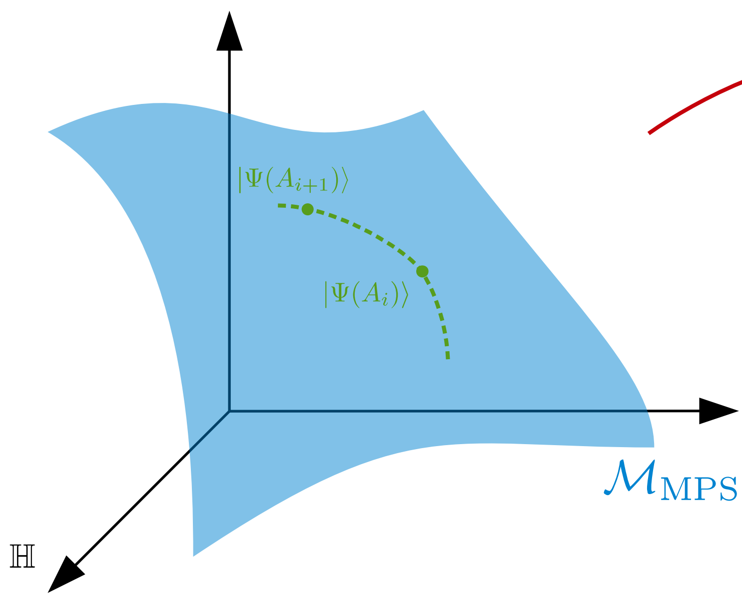
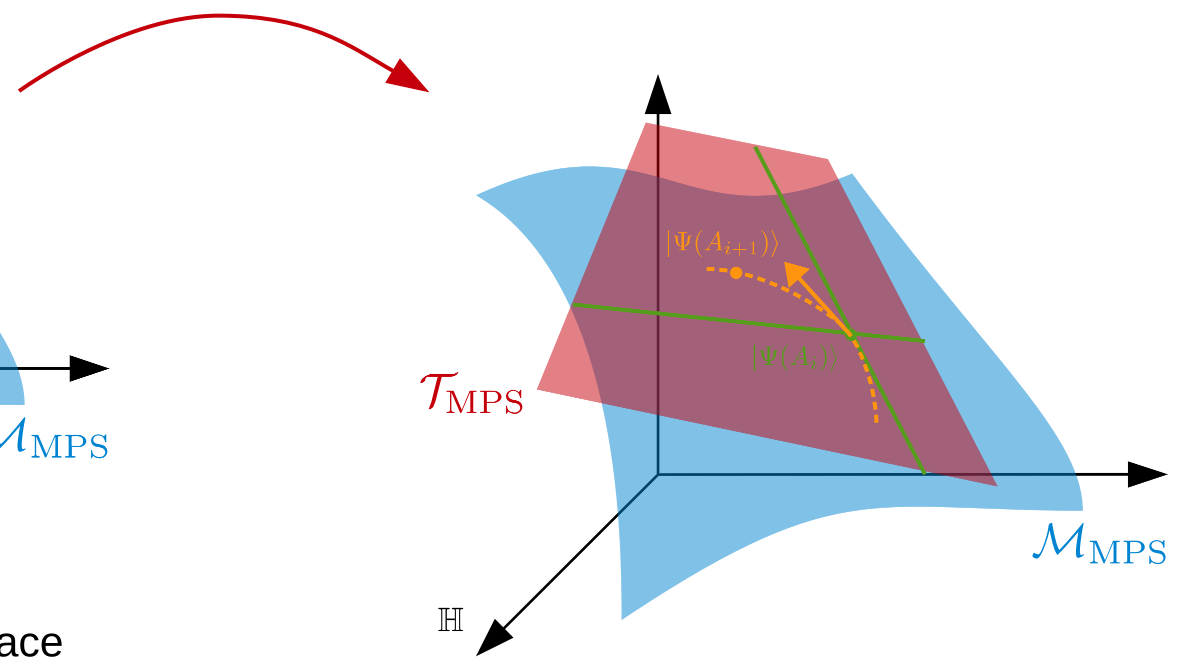
Variational optimization of MPS

Variational optimization of MPS tensor amounts to

$$\min_A \frac{\langle \Psi(A)| \, H \, |\Psi(A)\rangle}{\langle \Psi(A)|\Psi(A)\rangle}.$$

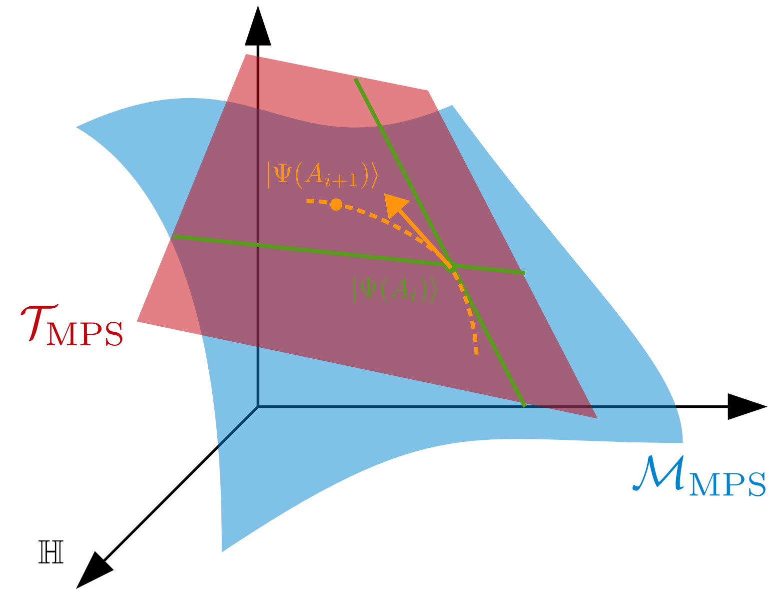
→ find a path through the manifold towards the variational optimum





The correct direction on the tangent space is provided by the energy gradient

Variational optimization of MPS



Variational optimization of MPS tensor amounts to

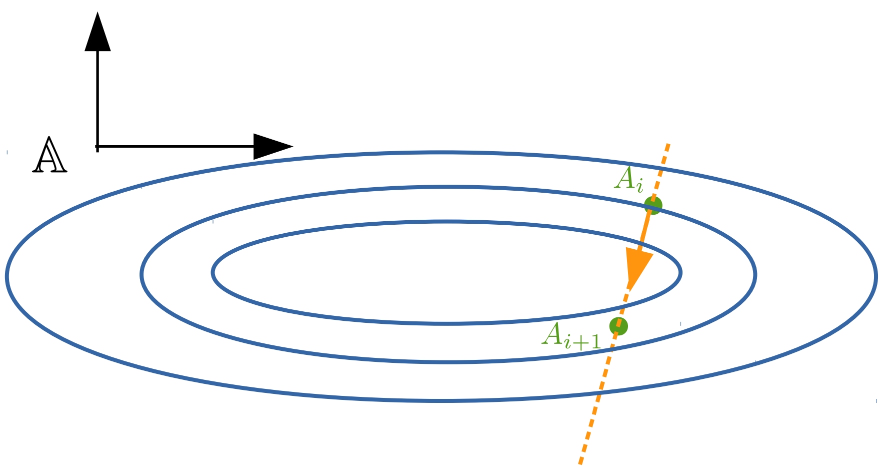
$$\min_A \frac{\langle\Psi(A)|\, H\, |\Psi(A)\rangle}{\langle\Psi(A)|\Psi(A)\rangle}.$$

→ find a path through the manifold towards the variational optimum

The correct direction on the tangent space is provided by the energy gradient

→ steepest descent

$$A_{i+1} = A_i - \alpha g$$



→ conjugate gradient, quasi-newton, hessian-based methods

→ numerical optimization on the manifold

Variational optimization of MPS

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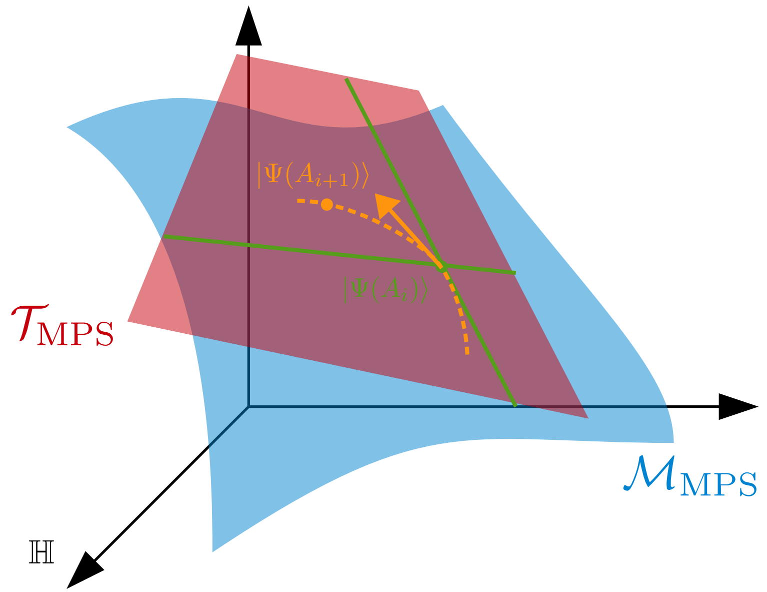
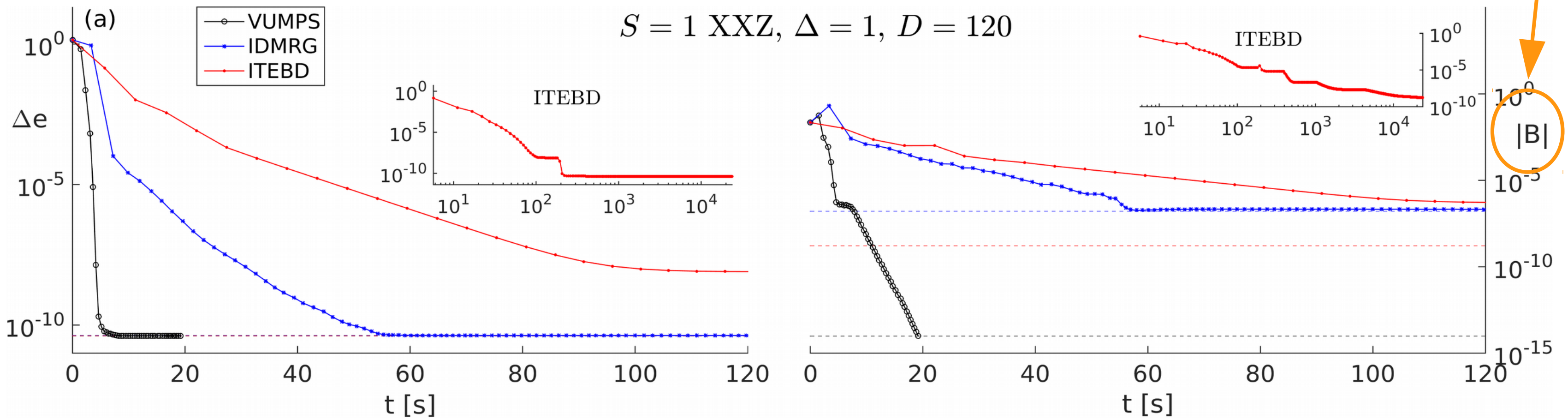


size of the gradient



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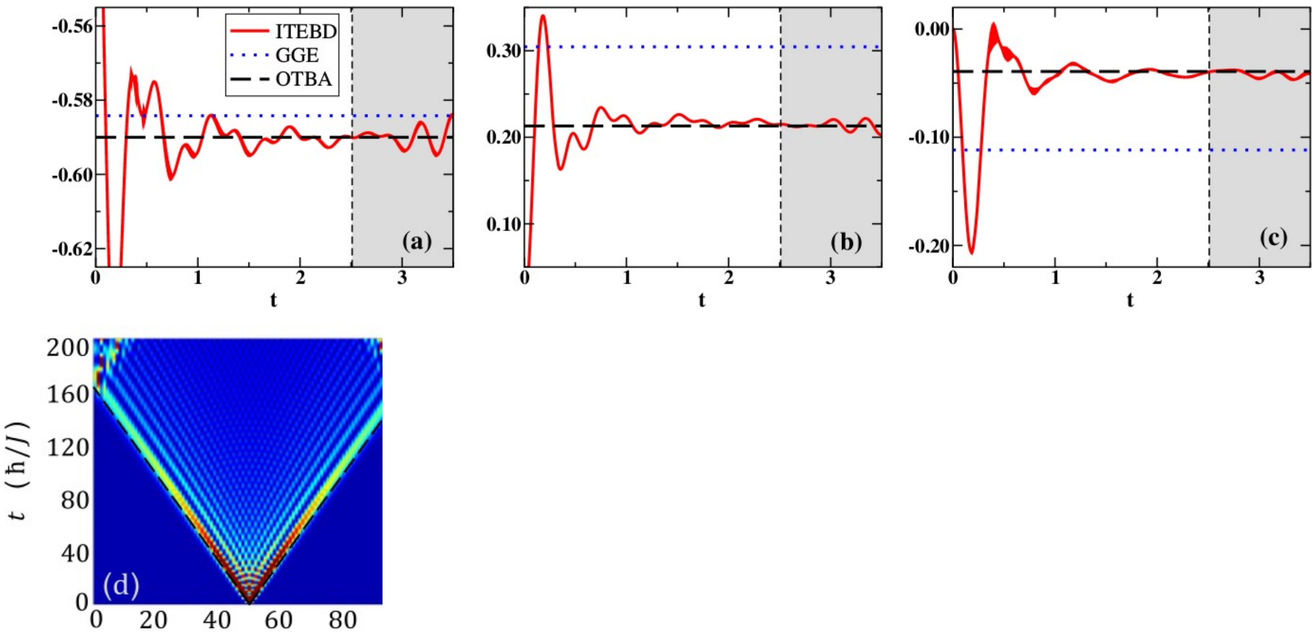
Time-dependent variational principle

The ground state of a given model Hamiltonian
is only the starting point

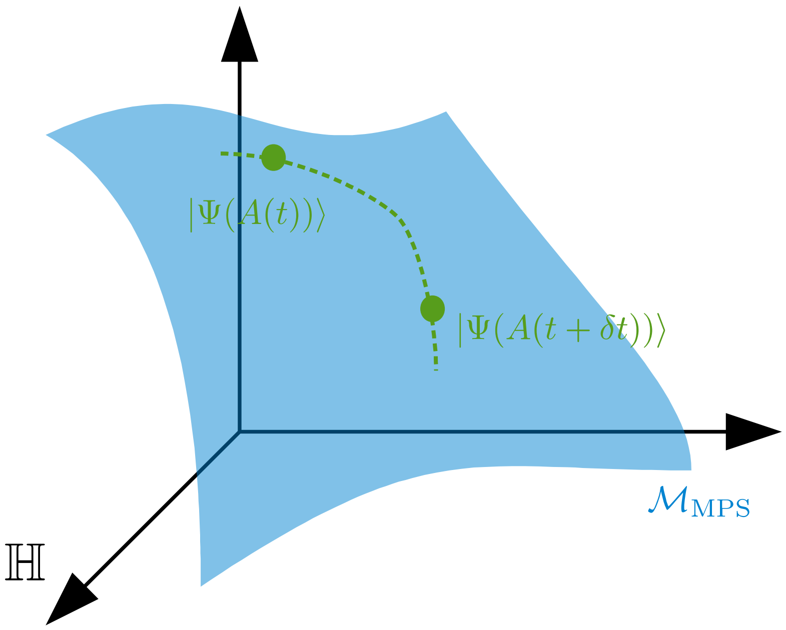
→ What about time evolution?



→ Straightforward option is using TEBD

Time-dependent variational principle

make MPS tensor time-dependent $|\Psi(A(t))\rangle$

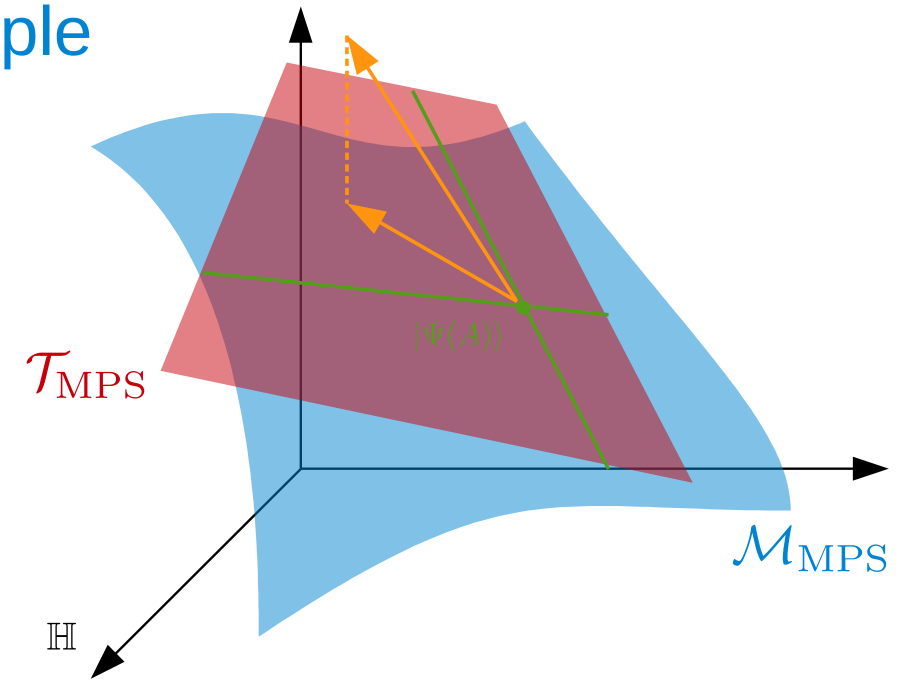


flow equation for the tensor

$$\dot{A}(t) = f(A(t))$$

→ How do we arrive at a flow equation that is optimal in a variational way?

Time-dependent variational principle



Start from Schrödinger equation

$$i\frac{\partial}{\partial t}|\Psi(A)\rangle = H|\Psi(A)\rangle$$

→ the right-hand side points out of the manifold!

Time-dependent variational principle (TDVP):

project time evolution onto the tangent space

$$i\frac{\partial}{\partial t}|\Psi(A(t))\rangle = P_{|\Psi(A(t))\rangle} H|\Psi(A(t))\rangle$$

The linear Schrödinger equation in full Hilbert space is transformed into a highly non-linear differential equation for the MPS tensor

$$\dot{A}(t) = f(A(t))$$

→ integrate flow equation numerically (Euler, Runge-Kutta, ...)

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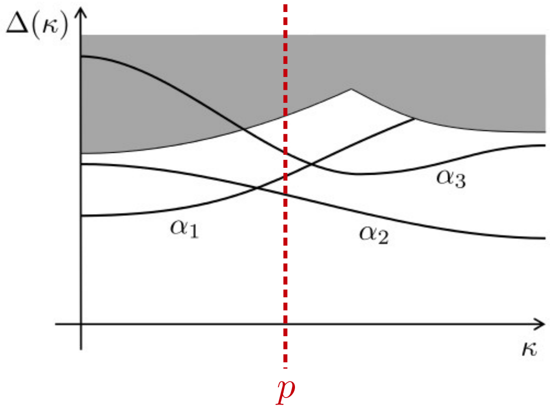
Quasiparticle excitations

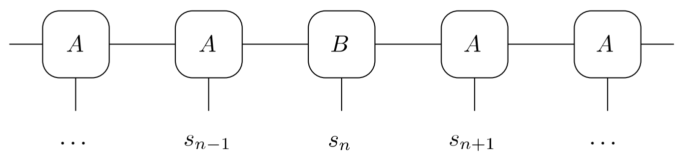
We want to target isolated branches in the excitation spectrum of generic spin chains

we can think of these excitations as quasiparticles on a strongly-correlated background state



Tangent space ansatz for elementary excitations with momentum

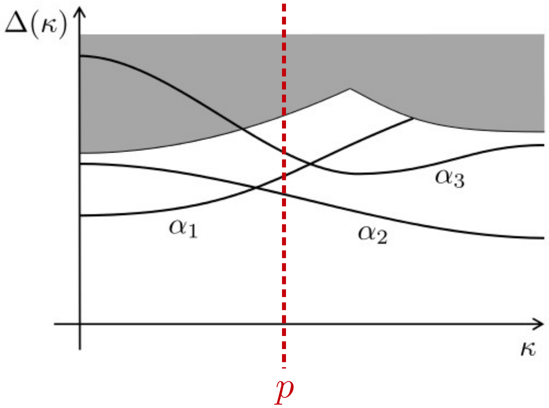
$$|\Phi_p(B)\rangle = \sum_n \mathrm{e}^{ipn} \ldots$$



“boosted” tangent vector

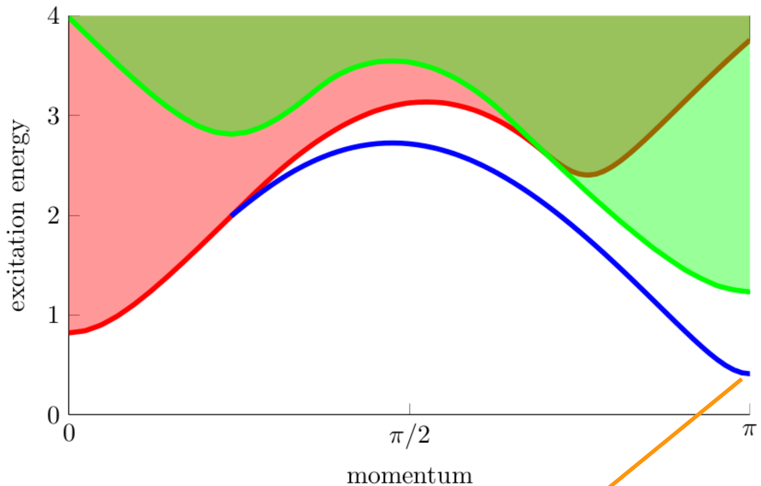
Optimize for tensor B

Quasiparticle excitations



We want to target isolated branches in the excitation spectrum of generic spin chains

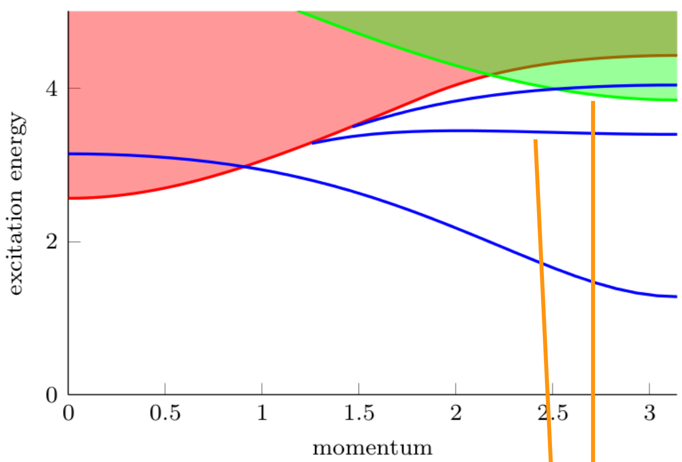
example: spin-1 Heisenberg chain



Haldane gap

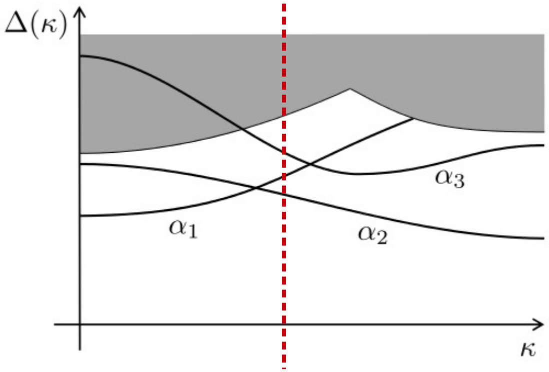
$$\Delta \approx 0.41047924871$$

example: spin-1/2 ladder

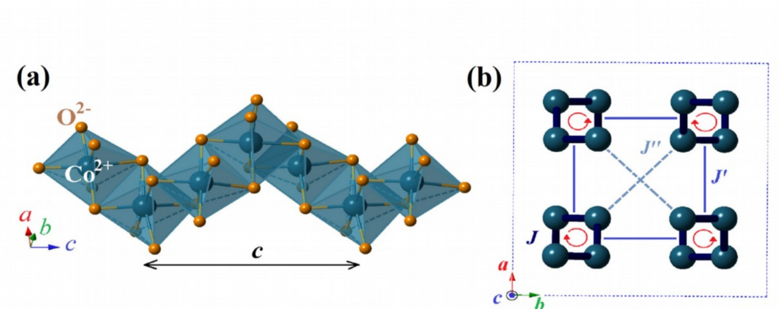


compute dispersion of bound states

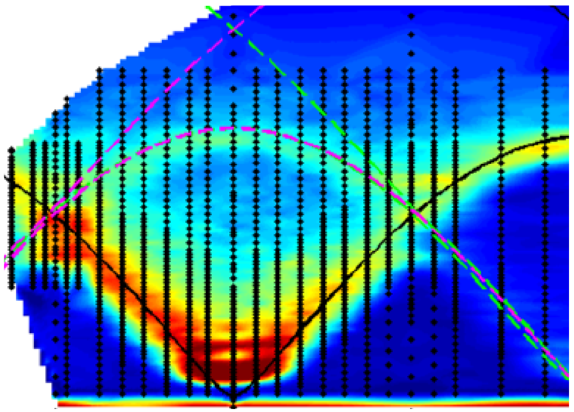
Quasiparticle excitations

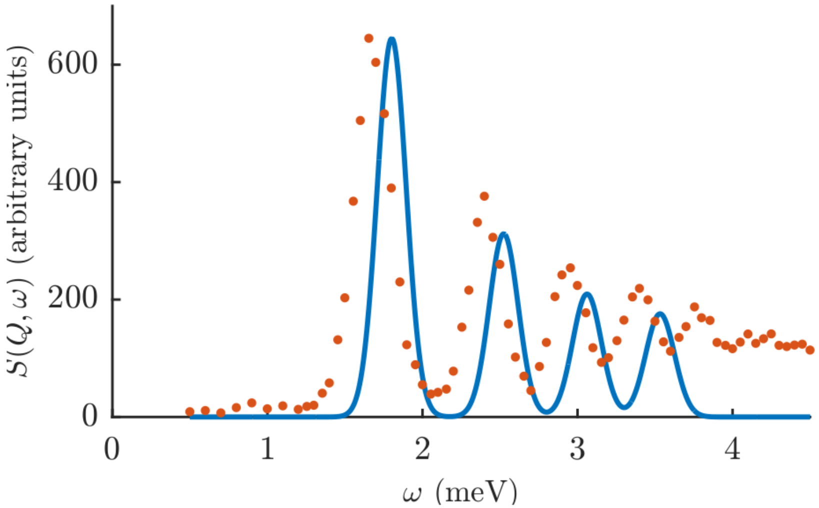


Confinement of spinons in quasi-1D Heisenberg magnet ($SrCo_2V_2O_8$)



Neutron-scattering experiments





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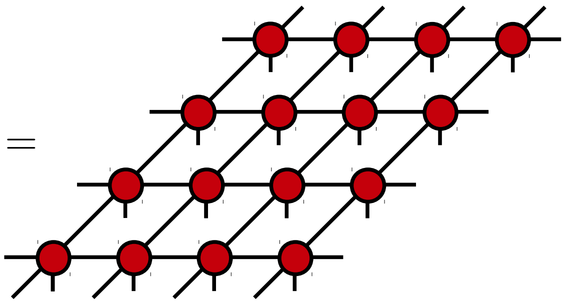
MPS construction is easily generalized to two dimensions

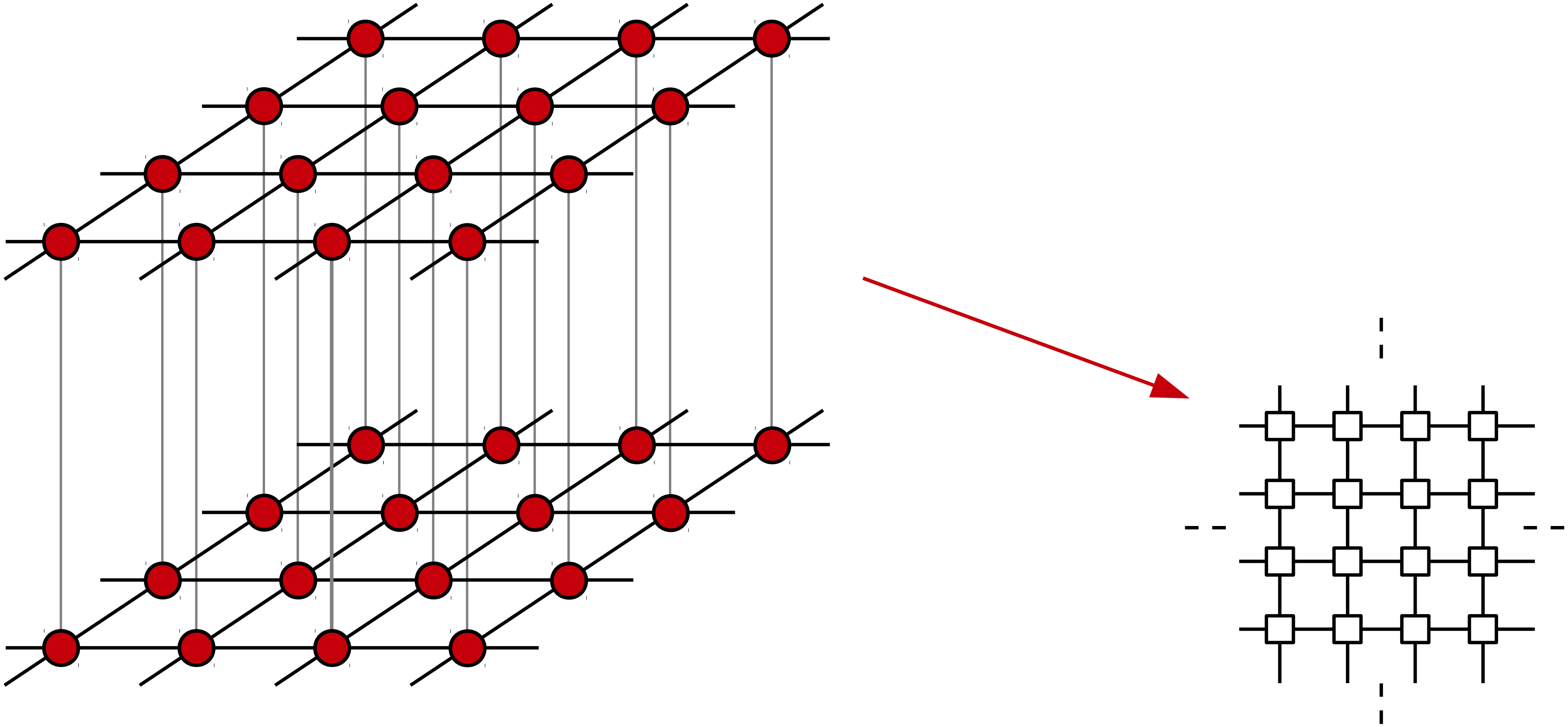
$$|\Psi(A)\rangle =$$



What about algorithms for PEPS?

Outlook: PEPS

Problem 1: Computing the norm of a PEPS is a hard problem



Outlook: PEPS

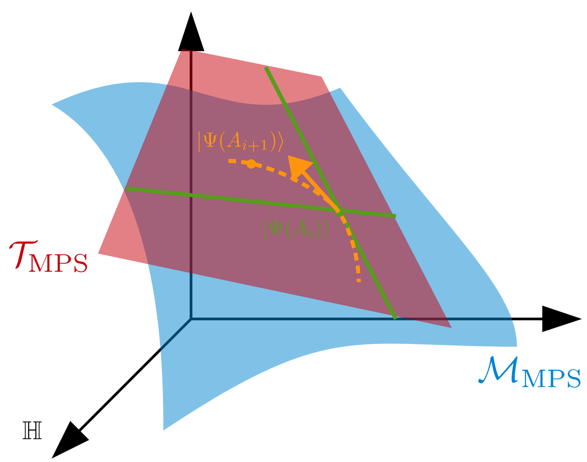
Problem 2: There are no canonical forms for PEPS

→ there is no easy algorithm for truncating the bond in a PEPS

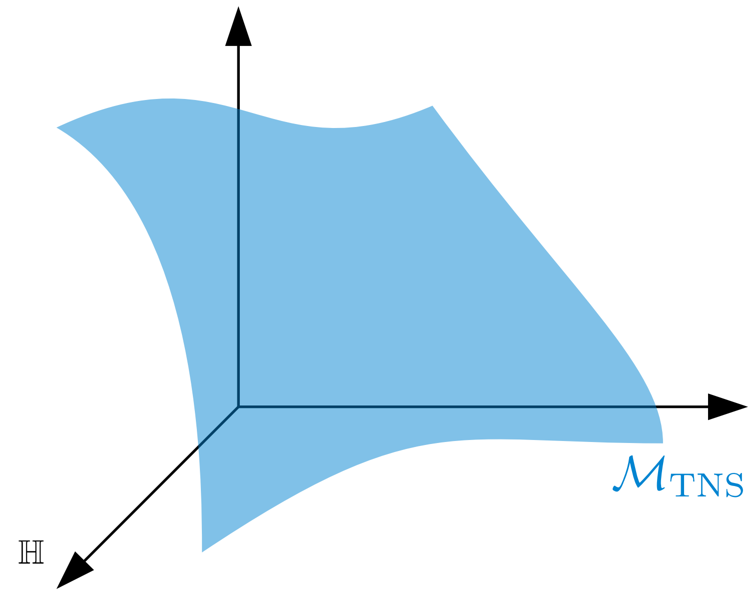
→ fixed-point algorithms are a lot more complicated

Full-update optimization: variation of iTEBD algorithm

Variational optimization ~ tangent-space method

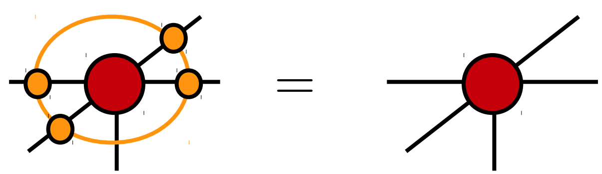


Outlook: PEPS

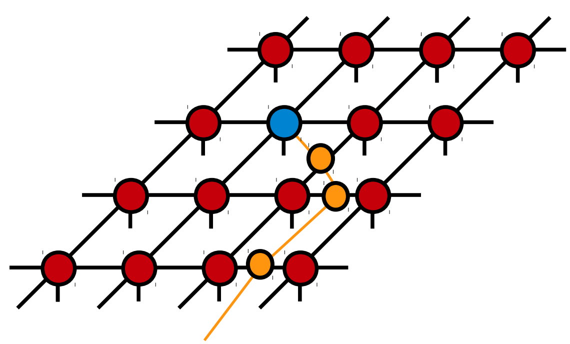


BUT: PEPS are a lot richer than MPS

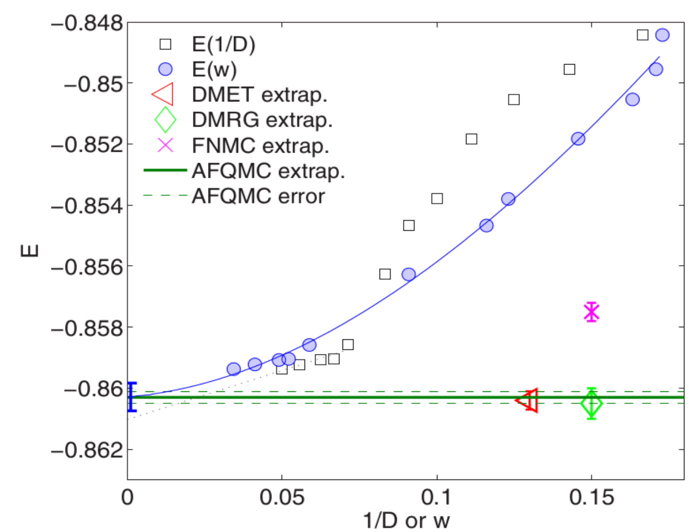
- PEPS can represent critical states
- PEPS have topological properties



- PEPS can host anyonic excitations



- PEPS simulations are competitive with other state-of-the-art numerical methods on challenging problems in two-dimensions



P. Corboz (2016)