Networking tensor networks:
many-body systems and simulations
May 14, 2012

(Differential) Geometry of Matrix Product States

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Motivation

Tangent space of the manifold of MPS:

- time-dependence: Phys. Rev. Lett. 107, 070601 (2011)
- elementary excitations: Phys. Rev. B 85, 100408(R) (2012)
- spectral functions (?)

Geometry of MPS

Better (more rigorous) understanding of what we have done

New insight into what else can be done

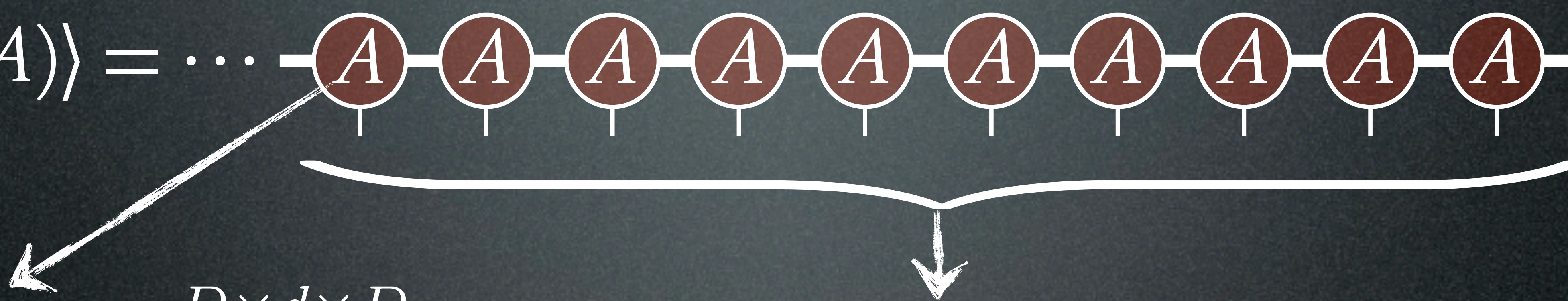
Outline

- Fiber bundle structure of MPS
- MPS tangent space and the need for a principle bundle connection
- Riemannian geometry of MPS
- Time-dependent variational principle and Hamiltonian dynamics
- Excitations and spectral functions
- Generalizations and outlook

Fiber bundle structure of Matrix Product States

Uniform matrix product states:

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



$\cdots$

$\mathbb{A}_{\mathrm{MPS}} = \mathbb{C}^{D\times d\times D}$

$\mathbb{H}$

Holomorphic map:

$$\Psi : \mathbb{A}_{\mathrm{MPS}} \to \mathbb{H} : A \mapsto |\Psi(A)\rangle$$

Variational set: (closed topological space)

$$\overline{\mathcal{M}}_{\mathrm{MPS}} = \left\{ |\Psi(A)\rangle \,|\, A \in \mathbb{A}_{\mathrm{MPS}} \right\}$$

Fiber bundle structure of Matrix Product States

Gauge invariance of MPS: $|\Psi(A)\rangle = |\Psi(A^G)\rangle$

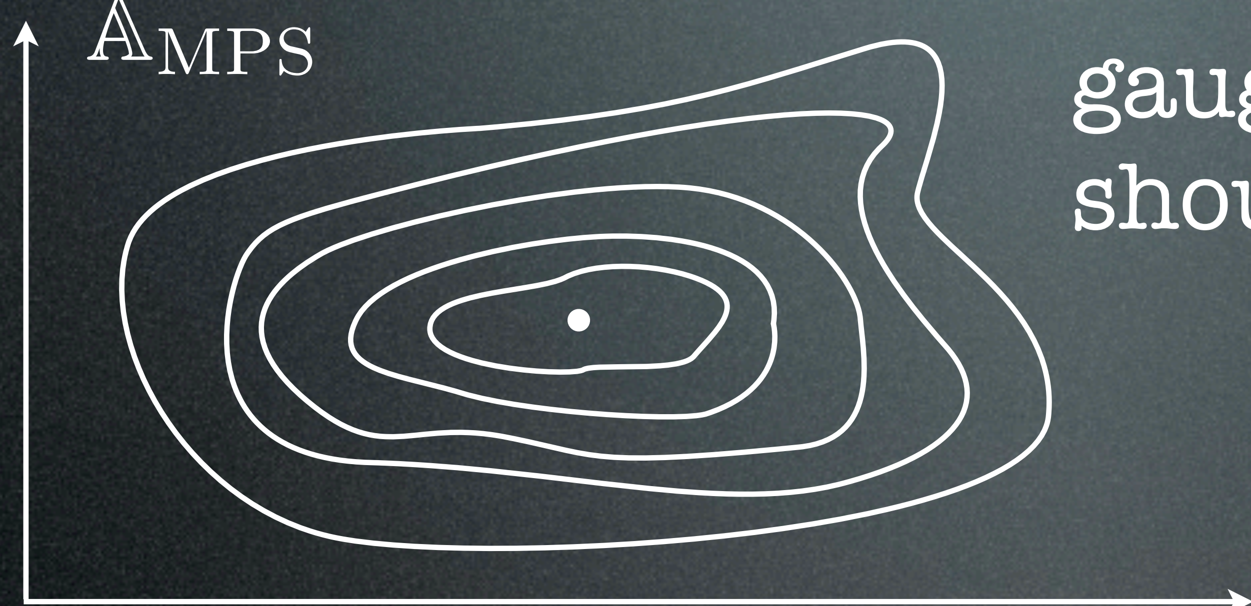
$\mathsf{G}_{\text{MPS}} = \mathsf{GL}(D, \mathbb{C})$

(Right) group action:

$$\Gamma\colon \mathbb{A}_{\text{MPS}} \times \mathsf{G}_{\text{MPS}} \to \mathbb{A}_{\text{MPS}} \colon (A, G) \mapsto \Gamma(A, G) = A^G$$

with $\Gamma\big(\Gamma(A, G_1), G_2\big) = \Gamma(A, G_1 G_2)$

Fiber bundle structure of Matrix Product States



gauge orbits:
should all look similar

$$\Downarrow$$

Free action:

- remove singular points:

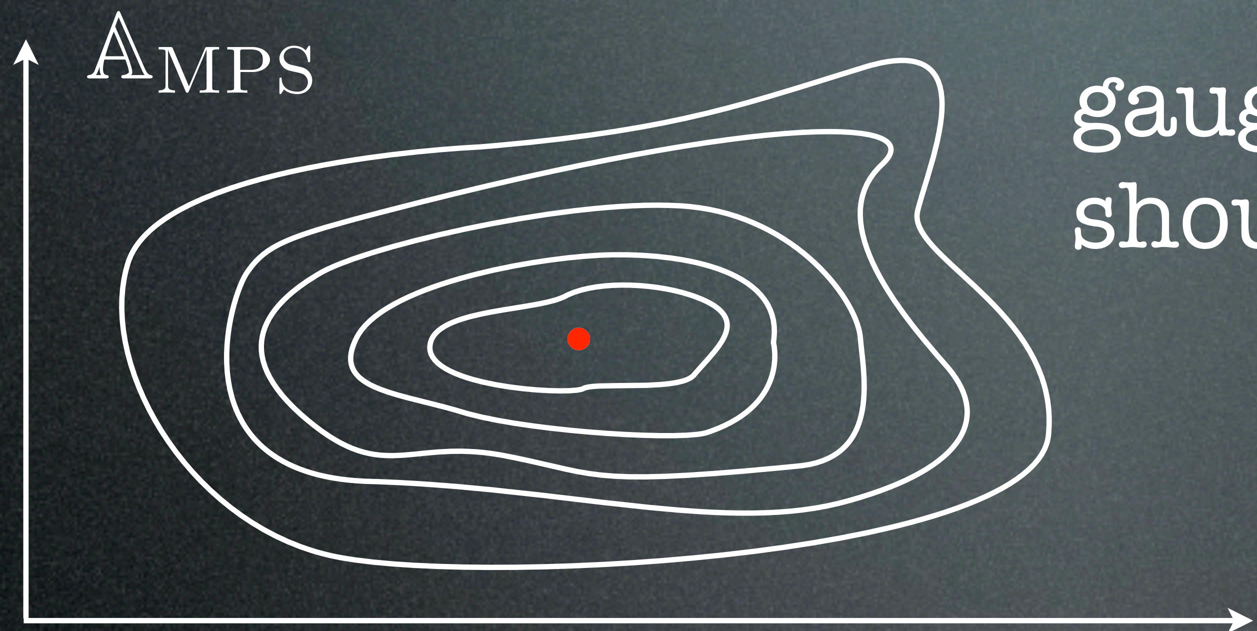
$$\mathbb{A}_{\text{MPS}} \to \mathcal{A}_{\text{MPS}}$$

- remove kernel of the group:

$$\mathsf{S}_{\text{MPS}} = \mathsf{G}_{\text{MPS}}/\mathsf{GL}(1,\mathbb{C}) = \mathsf{PGL}(D,\mathbb{C})$$

Proper action: technical condition that is fulfilled

Fiber bundle structure of Matrix Product States



gauge orbits:
should all look similar

$$\Downarrow$$

Free action:
- remove singular points:

$$\mathbb{A}_{\mathrm{MPS}} \to \mathcal{A}_{\mathrm{MPS}}$$

'injective MPS'

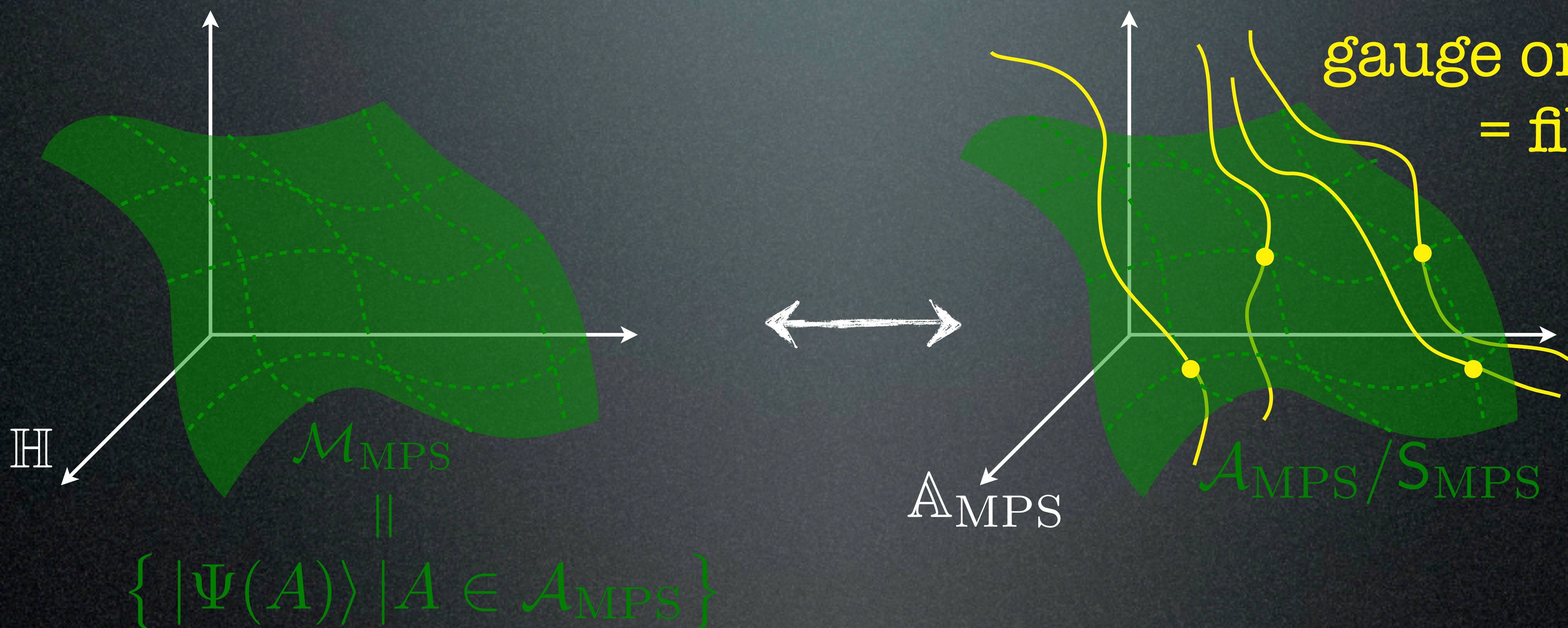
- remove kernel of the group:

$$\mathsf{S}_{\mathrm{MPS}} = \mathsf{G}_{\mathrm{MPS}}/\mathsf{GL}(1,\mathbb{C}) = \mathsf{PGL}(D,\mathbb{C})$$

projective linear group

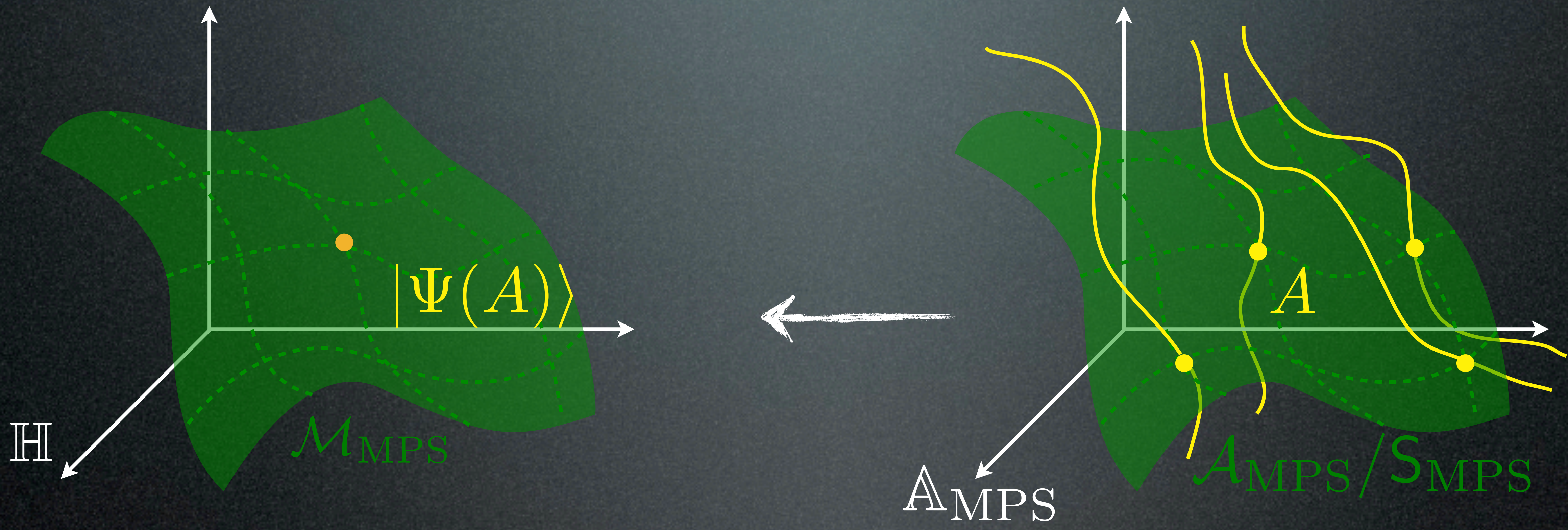
Proper action: technical condition that is fulfilled

Fiber bundle structure of Matrix Product States



- $\Psi : \mathcal{A}_{\mathrm{MPS}} \to \mathcal{M}_{\mathrm{MPS}}$ is a principal fiber bundle with structure group $\mathsf{S}_{\mathrm{MPS}}$
- $\mathcal{M}_{\mathrm{MPS}}$ is a complex manifold that is biholomorphic to $\mathcal{A}_{\mathrm{MPS}}/\mathsf{S}_{\mathrm{MPS}}$

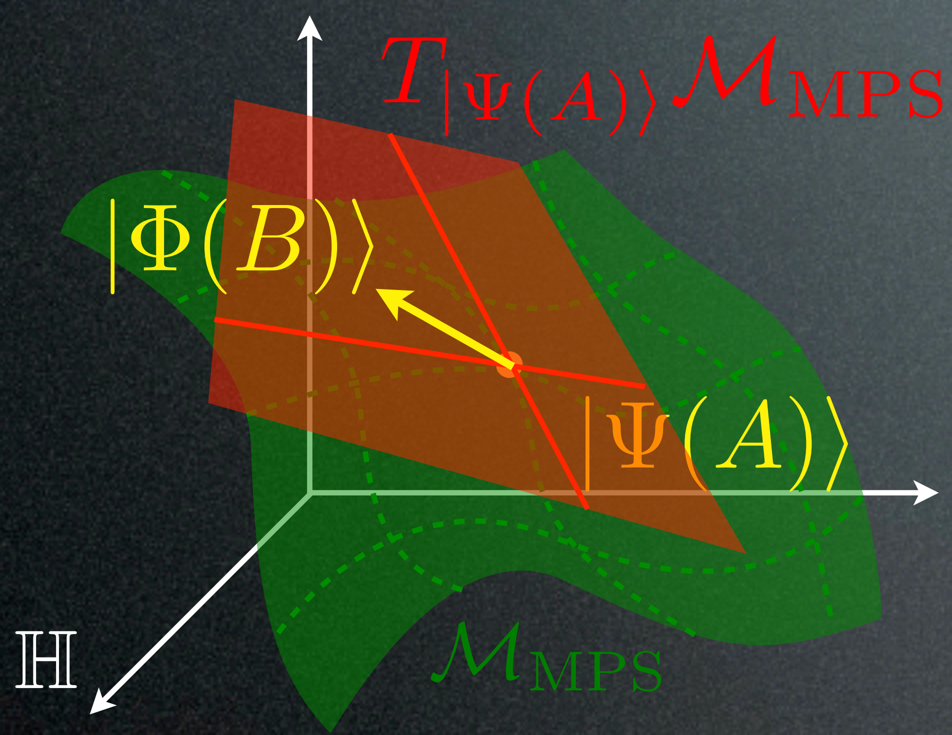
Tangent space of Matrix Product States

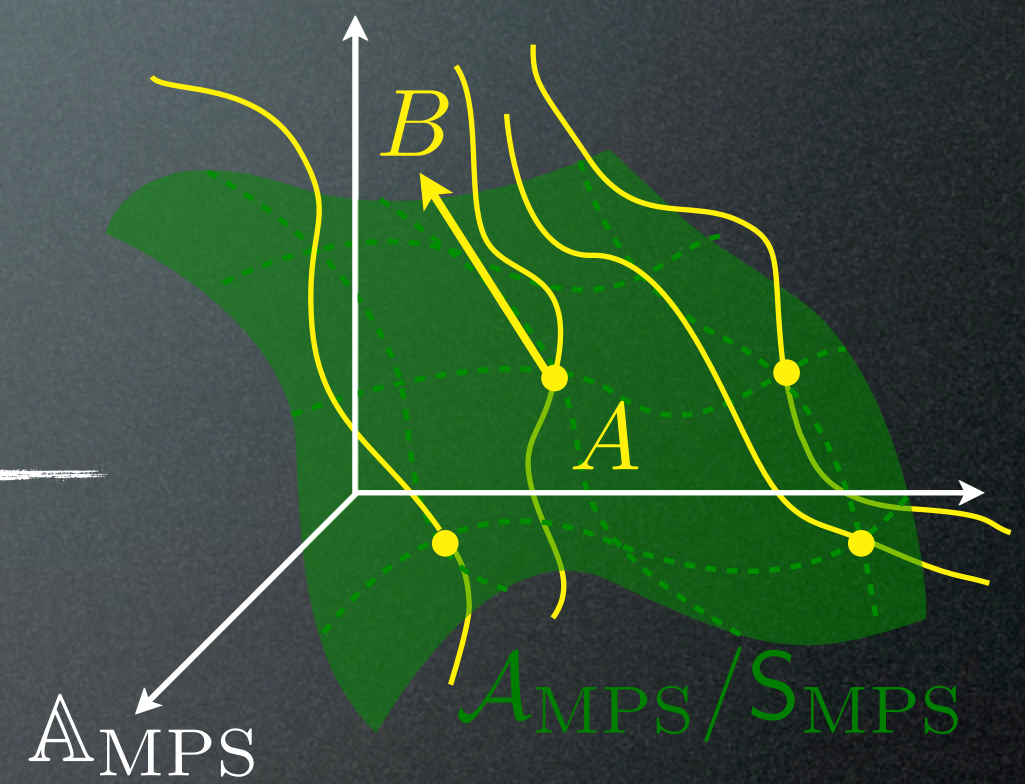


Tangent map $\mathrm{d}\Psi$ is a homomorphism between $T_{|\Psi(A)\rangle}\mathcal{A}_{\mathrm{MPS}}$ and $T_A\mathcal{A}_{\mathrm{MPS}} = \mathbb{A}_{\mathrm{MPS}}$

(actually: holomorphic part of tangent space)

Tangent space of Matrix Product States





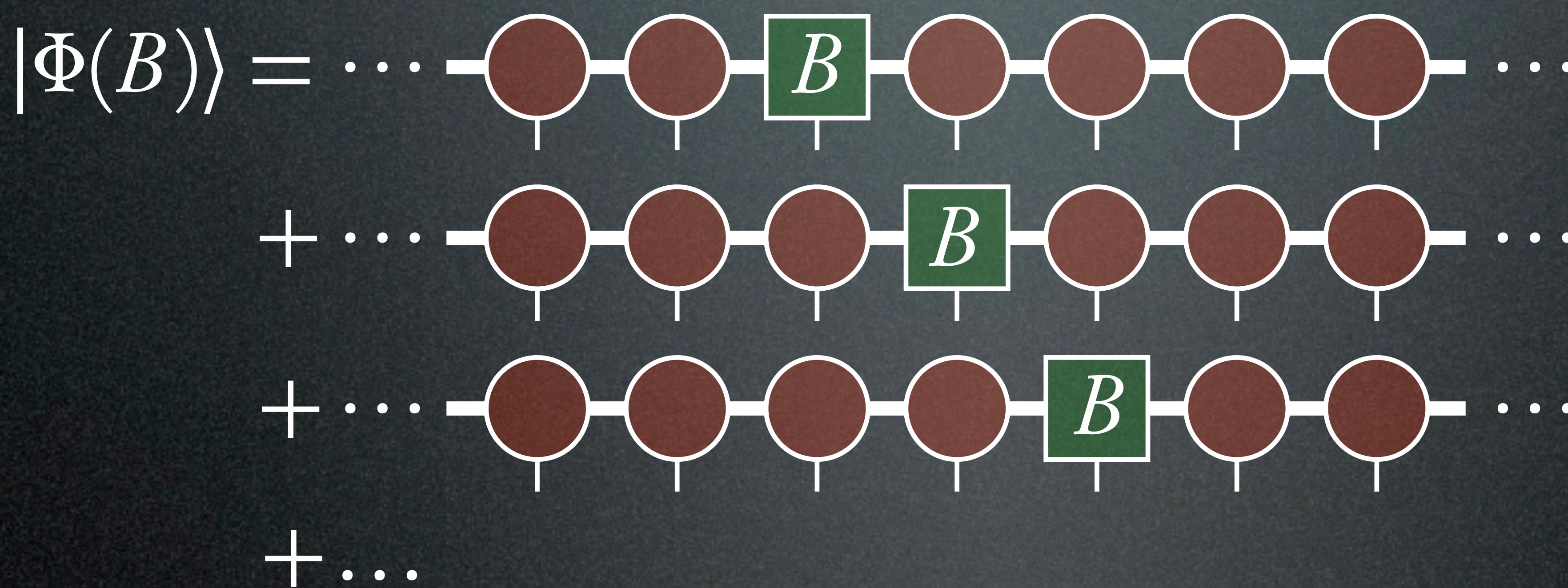
$T_A\mathcal{A}_{\mathrm{MPS}} = \mathbb{A}_{\mathrm{MPS}}$

Tangent map $\mathrm{d}\Psi$ is a homomorphism between $T_{|\Psi(A)\rangle}\mathcal{A}_{\mathrm{MPS}}$ and $T_A\mathcal{A}_{\mathrm{MPS}} = \mathbb{A}_{\mathrm{MPS}}$

(actually: holomorphic part of tangent space)

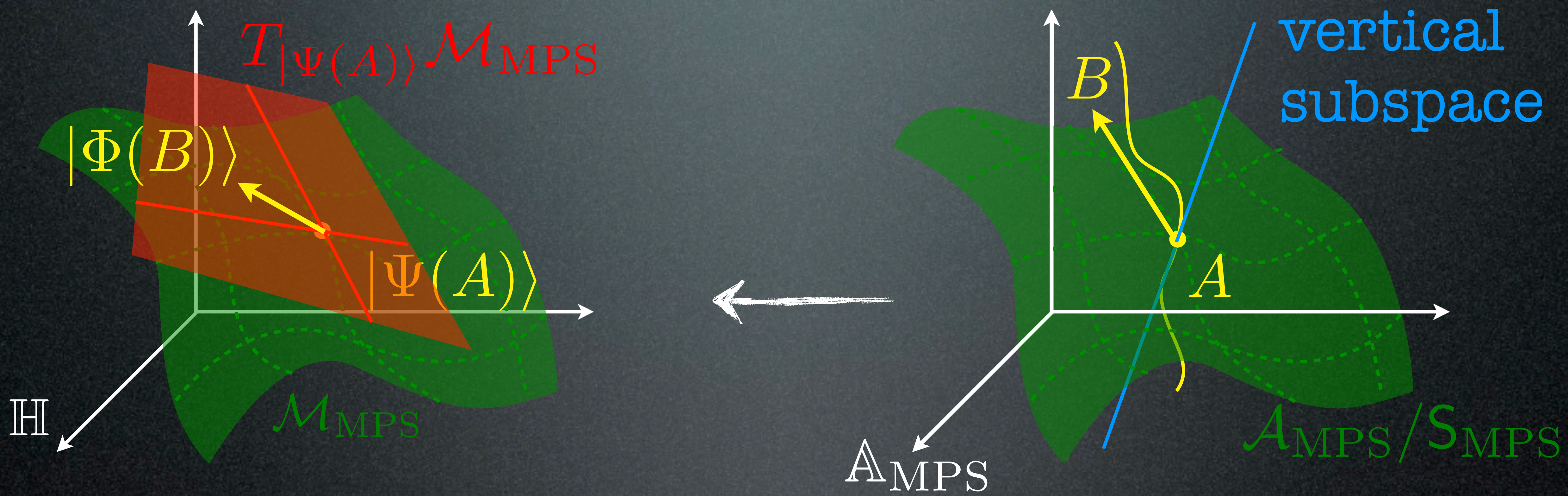
Tangent space of Matrix Product States

Tangent vectors: $B^i \, |\partial_i \Psi(A)\rangle = |\Phi(B)\rangle \quad (i = 1, \ldots, dD^2)$



$$\mathrm{d}\Psi_A : T_A \mathcal{A}_{\mathrm{MPS}} \to T_{|\Psi(A)\rangle} \mathcal{M}_{\mathrm{MPS}} : B \mapsto |\Phi(B)\rangle$$

Tangent space of Matrix Product States



$$T_A\mathcal{A}_{\mathrm{MPS}} = \mathbb{A}_{\mathrm{MPS}}$$

$$\mathbb{N}^A = \mathrm{Ver}\ T_A\mathcal{A}_{\mathrm{MPS}} = \ker \mathrm{d}\Psi_A \subset \mathbb{A}_{\mathrm{MPS}}$$

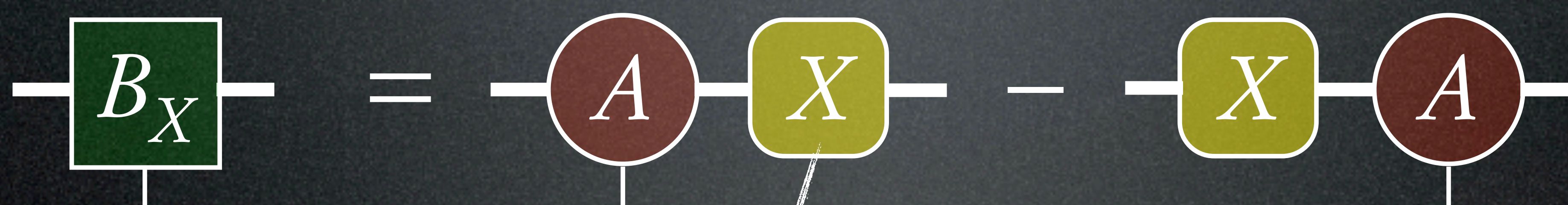
$$\forall B' \in \mathbb{N}^A : |\Phi(B)\rangle = |\Phi(B+B')\rangle = |\Phi(B)\rangle + \underbrace{|\Phi(B')\rangle}_{=0}$$

Tangent space of Matrix Product States

Gauge invariance of MPS: $|\Psi(A)\rangle = |\Psi(A_G)\rangle$

$G = \exp(\epsilon X)$

Gauge invariance of tangent vectors: $|\Phi(B_X)\rangle = 0$



$$\mathbb{N}^A \equiv \mathfrak{g}_{\mathrm{MPS}} = \mathfrak{gl}(D, \mathbb{C}) = \mathbb{C}^{D\times D}$$

Tangent space of Matrix Product States

$\Rightarrow$ **Gauge fixing prescription:** fix D^2 components

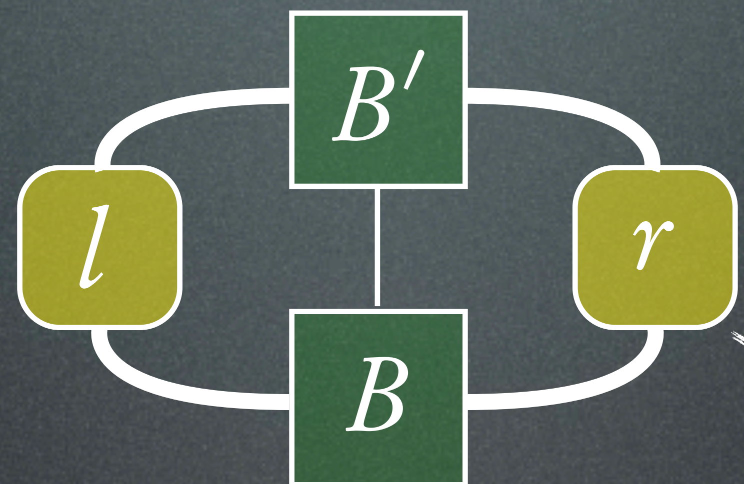
with

$$T_A\mathcal{A}_{\mathrm{MPS}} = \mathrm{Ver}\,T_A\mathcal{A}_{\mathrm{MPS}} \oplus \underbrace{\mathrm{Hor}\,T_A\mathcal{A}_{\mathrm{MPS}}}_{\text{defined via principal bundle connection}}$$

Riemannian geometry with MPS

Metric of the MPS manifold:

$$\langle \Phi(B) | \Phi(B') \rangle \sim$$



non-injective MPS are singular points

$$g_{\bar{\imath},j} = \langle \partial_{\bar{\imath}} \Psi(\overline{A}) | \partial_j \Psi(A) \rangle = \partial_{\bar{\imath}} \partial_j K(\overline{A}, A)$$

with $\quad K(A, A) = \langle \Psi(A) | \Psi(A) \rangle$

$\Rightarrow$ Kahler manifold

Riemannian geometry with MPS

Levi-Civita connection:

$$\Gamma_{i,j}{}^{k} = g^{k,\overline{m}} \langle \partial_{\overline{m}} \Psi | \partial_i \partial_j \Psi \rangle$$

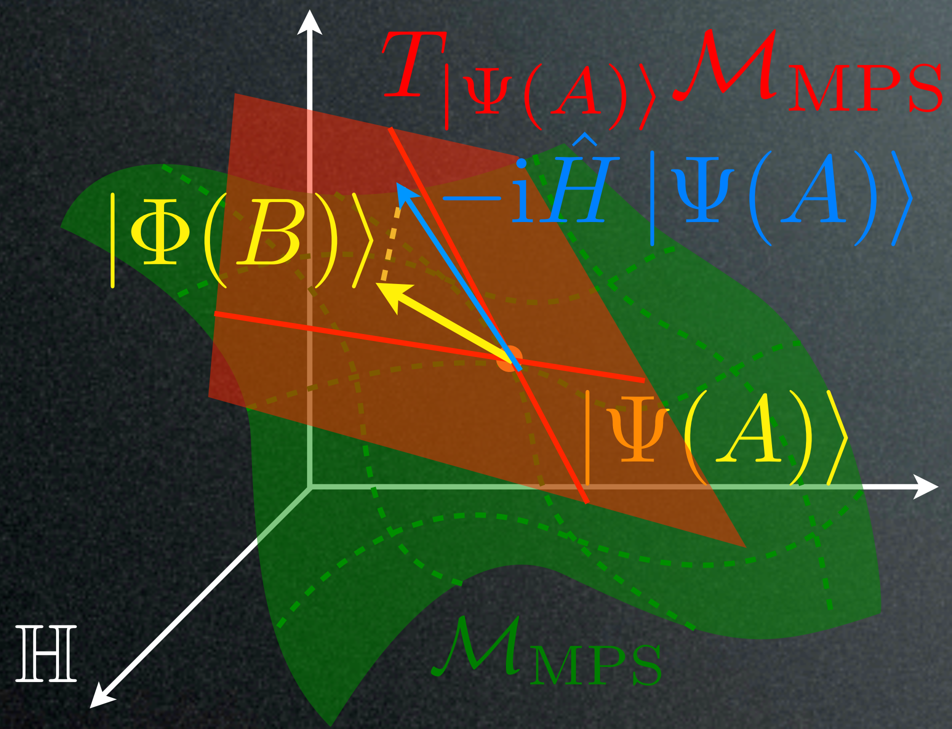
covariant derivate

$$\begin{aligned} \nabla_i \nabla_j \left| \Psi \right\rangle &= \left| \partial_i \partial_j \Psi(A) \right\rangle - \left| \partial_k \Psi \right\rangle g^{k,\overline{m}} \langle \partial_{\overline{m}} \Psi | \partial_i \partial_j \Psi(A) \rangle \\ &= (\hat{1} - \hat{P}_T) \left| \partial_i \partial_j \Psi(A) \right\rangle \end{aligned}$$

Riemann curvature tensor:

$$R_{i,\bar{j},k,\bar{l}} = \langle \partial_{\bar{j}} \partial_{\bar{l}} | (\hat{1} - \hat{P}_T) | \partial_i \partial_k \Psi \rangle$$

Time-dependent variational principle



Dirac, 1930

Exact time evolution in Hilbert space:

$$\frac{\mathrm{d}}{\mathrm{d}t}\,|\Psi(t)\rangle = -\mathrm{i}\hat{H}\,|\Psi(t)\rangle$$

Projection onto the tangent plane:

$$\langle \partial_{\bar{\imath}}\Psi(\overline{A(t)})|\partial_j\Psi(A(t))\rangle\,\dot{A}^j(t) = -\mathrm{i}\,\langle \partial_{\bar{\imath}}\Psi(\overline{A(t)})|\hat{H}|\Psi(A(t))\rangle$$

$$\Rightarrow \dot{A}^j(t) = -\mathrm{i}g^{j,\bar{\imath}}\,\langle \partial_{\bar{\imath}}\Psi(\overline{A(t)})|\hat{H}|\Psi(A(t))\rangle$$

Time-dependent variational principle

$$O(\overline{A}, A) = \langle \Psi(\overline{A}) | \hat{O} | \Psi(A) \rangle$$

$$H(\overline{A}, A) = \langle \Psi(\overline{A}) | \hat{H} | \Psi(A) \rangle$$

$$\Rightarrow \frac{\mathrm{d}}{\mathrm{d}t} O(\overline{A(t)}, A(t)) = -\mathrm{i}(\partial_i O) g^{i,\bar{\jmath}} (\partial_{\bar{\jmath}} H) + \mathrm{i}(\partial_i H) g^{i,\bar{\jmath}} (\partial_{\bar{\jmath}} O)$$

$$= -\mathrm{i}\{O, H\}$$

Poisson bracket

Hamiltonian dynamics

Kahler manifolds $\subset$ symplectic manifold

Time-dependent variational principle

- TDVP evolution never leaves $\mathcal{M}_{\mathrm{MPS}}$:
  Linear differential equation in large space $\mathbb{H}$

  $\Updownarrow$

  Non-linear differential equation in $\mathcal{M}_{\mathrm{MPS}}$
- Inherently respects all symmetries:
  no Trotter decomposition $\Rightarrow$ no Trotter error
- Globally optimal, no truncation
- Quantum version of the Gross-Pitaevskii equation

Linearized TDVP

Variational optimum satisfies

$$\langle \Phi(\overline{B}) | \hat{H} | \Psi(A^*) \rangle \sim \overline{B}^{\bar{\imath}} \partial_{\bar{\imath}} H(A^*) = 0$$

$\Rightarrow$ Steady state solution of TDVP equations

Linearize TDVP around ground state:

$$A(t) = A^* + \eta B(t)$$

$\Rightarrow$ First order linear differential equation in $B(t)$ and $\overline{B(t)}$:

$$B(t) = B_+ \mathrm{e}^{-\mathrm{i}\omega t} + B_- \mathrm{e}^{+\mathrm{i}\omega t}$$

Linearized TDVP

$$\omega \begin{bmatrix} \langle \partial_i \Psi(A^*) | \partial_j \Psi(A^*) \rangle & 0 \\ 0 & -\overline{\langle \partial_i \Psi(A^*) | \partial_j \Psi(A^*) \rangle} \end{bmatrix} \begin{bmatrix} {B_+}^j \\ \overline{{B_-}^j} \end{bmatrix}$$

$$= \begin{bmatrix} \langle \partial_i \Psi(A^*) | \hat{H} | \partial_j \Psi(A^*) \rangle & \langle \partial_i \partial_j \Psi(A^*) | \hat{H} | \Psi(A^*) \rangle \\ \overline{\langle \partial_i \partial_j \Psi(A^*) | \hat{H} | \Psi(A^*) \rangle} & \overline{\langle \partial_i \Psi(A^*) | \hat{H} | \partial_j \Psi(A^*) \rangle} \end{bmatrix} \begin{bmatrix} {B_+}^j \\ \overline{{B_-}^j} \end{bmatrix}$$

Linearized TDVP

$$\omega \begin{bmatrix} \langle \partial_i \Psi(A^*) | \partial_j \Psi(A^*) \rangle & 0 \\ \hline 0 & -\langle \partial_i \Psi(A^*) | \partial_j \Psi(A^*) \rangle \end{bmatrix} \begin{bmatrix} {B_+}^j \\ \hline {B_-}^j \end{bmatrix}$$

$$= \begin{bmatrix} \langle \partial_i \Psi(A^*) | \hat{H} | \partial_j \Psi(A^*) \rangle & \cancel{\langle \partial_i \partial_j \Psi(A^*) | \hat{H} | \Psi(A^*) \rangle} \\ \hline \cancel{\langle \partial_i \partial_j \Psi(A^*) | \hat{H} | \Psi(A^*) \rangle} & \langle \partial_i \Psi(A^*) | \hat{H} | \partial_j \Psi(A^*) \rangle \end{bmatrix} \begin{bmatrix} {B_+}^j \\ \hline {B_-}^j \end{bmatrix}$$

$$\Downarrow$$

$$\omega \, \langle \partial_i \Psi(A^*) | \partial_j \Psi(A^*) \rangle \, B^j = \langle \partial_i \Psi(A^*) | \hat{H} | \partial_j \Psi(A^*) \rangle \, B^j$$

Application of variational principle in
linear subspace $T_{|\Psi(A)\rangle}\mathcal{M}_{\mathrm{MPS}}$.

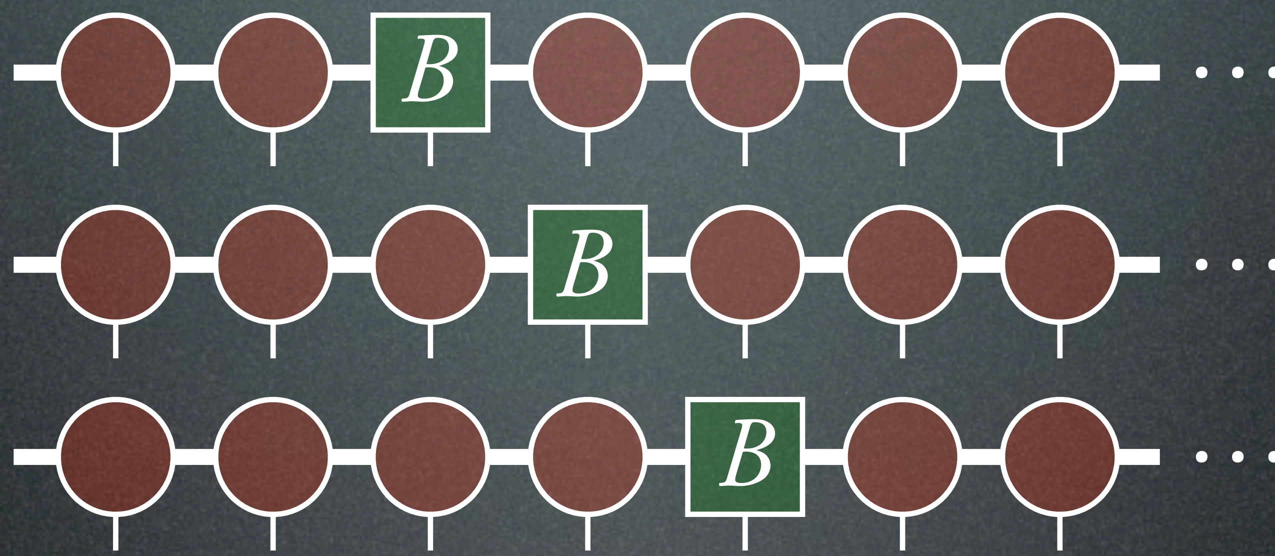
(Rayleigh - Ritz equations)

Ansatz for excitations

$|\Phi(B)\rangle = \cdots$

$+ \cdots$

$+ \cdots$



$+ \dots$

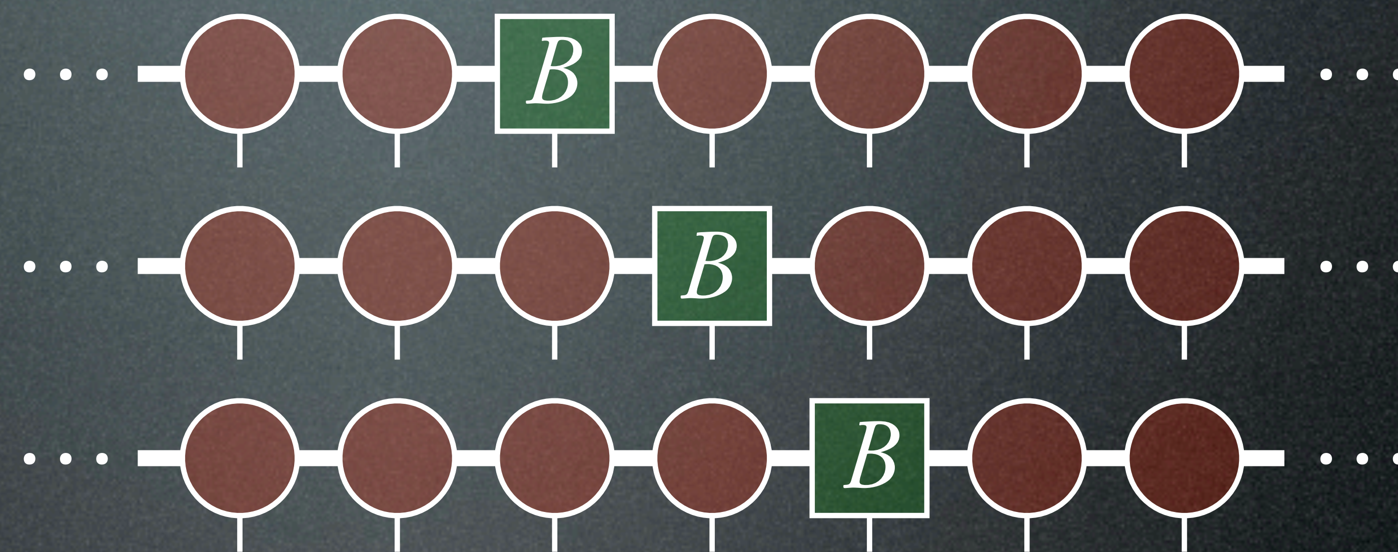
Ansatz for excitations

$$|\Phi(B)\rangle = \mathrm{e}^{ik(n-1)}$$

$$+\ \mathrm{e}^{ikn}$$

$$+\ \mathrm{e}^{ik(n+1)}$$

$$+\dots$$



$\Rightarrow$ Ansatz for excitations with momentum k

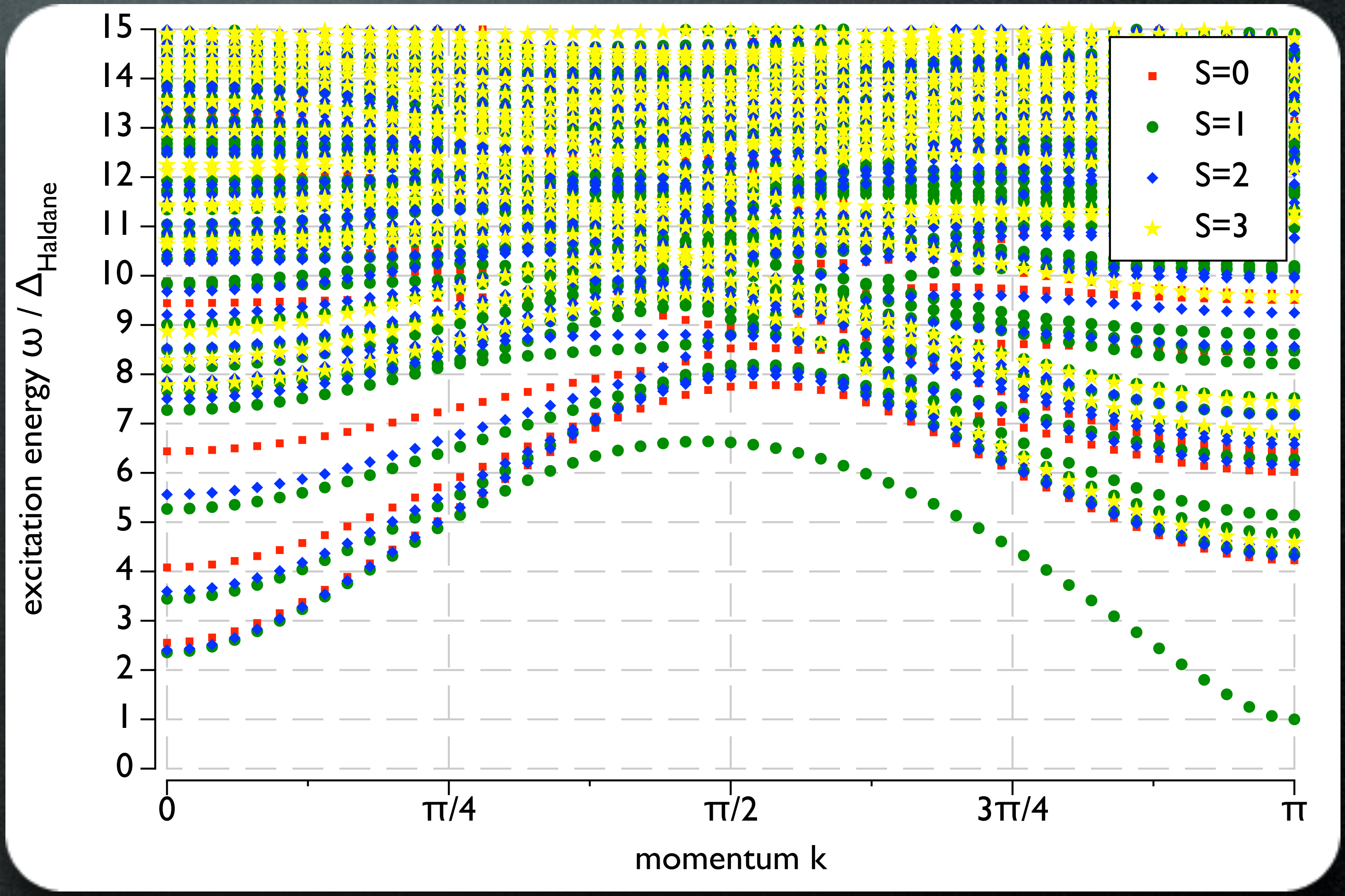
Combines:

- Östlund - Rommer ansatz
- Single-mode approximation (Feynman-Bijl ansatz)

Ansatz for excitations: dispersion relations

S=1 Heisenberg AFM: $\hat{H} = \sum_{n\in\mathbb{Z}} \hat{S}^x_n \hat{S}^x_{n+1} + \hat{S}^y_n \hat{S}^y_{n+1} + \hat{S}^z_n \hat{S}^z_{n+1}$

$D = 30$:



Efficient implementation:

$\Downarrow D = 208$

$\Delta_{\text{Haldane}} = 0.410479248463^{+6\times10^{-12}}_{-3\times10^{-12}}$

From excitations to spectral functions

$$S^{\alpha,\beta}(k,\omega) = \underbrace{\langle\Psi|}(\hat{O}^{\alpha}_{k})^{\dagger}\delta(\omega - \hat{H})\hat{O}^{\beta}_{k}\underbrace{|\Psi\rangle}$$

uniform MPS

From excitations to spectral functions

$$S^{\alpha,\beta}(k,\omega) = \underbrace{\langle\Psi|(\hat{O}_k^{\alpha})^{\dagger}}\delta(\omega - \hat{H})\underbrace{\hat{O}_k^{\beta}|\Psi\rangle}$$

MPS tangent vectors

$\Rightarrow$ no loss of spectral weight

From excitations to spectral functions

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MPS tangent vectors

$\Rightarrow$ no loss of spectral weight

$$S^{\alpha,\beta}(k,\omega) = \langle\Psi|(\hat{O}_k^{\alpha})^{\dagger}\hat{P}_{\mathbb{T}}\delta(\omega - \hat{H})\hat{P}_{\mathbb{T}}\hat{O}_k^{\beta}|\Psi\rangle$$
$$\approx \langle\Psi|(\hat{O}_k^{\alpha})^{\dagger}\delta(\omega - \hat{P}_{\mathbb{T}}\hat{H}\hat{P}_{\mathbb{T}})\hat{O}_k^{\beta}|\Psi\rangle$$

From excitations to spectral functions

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MPS tangent vectors

$\Rightarrow$ no loss of spectral weight

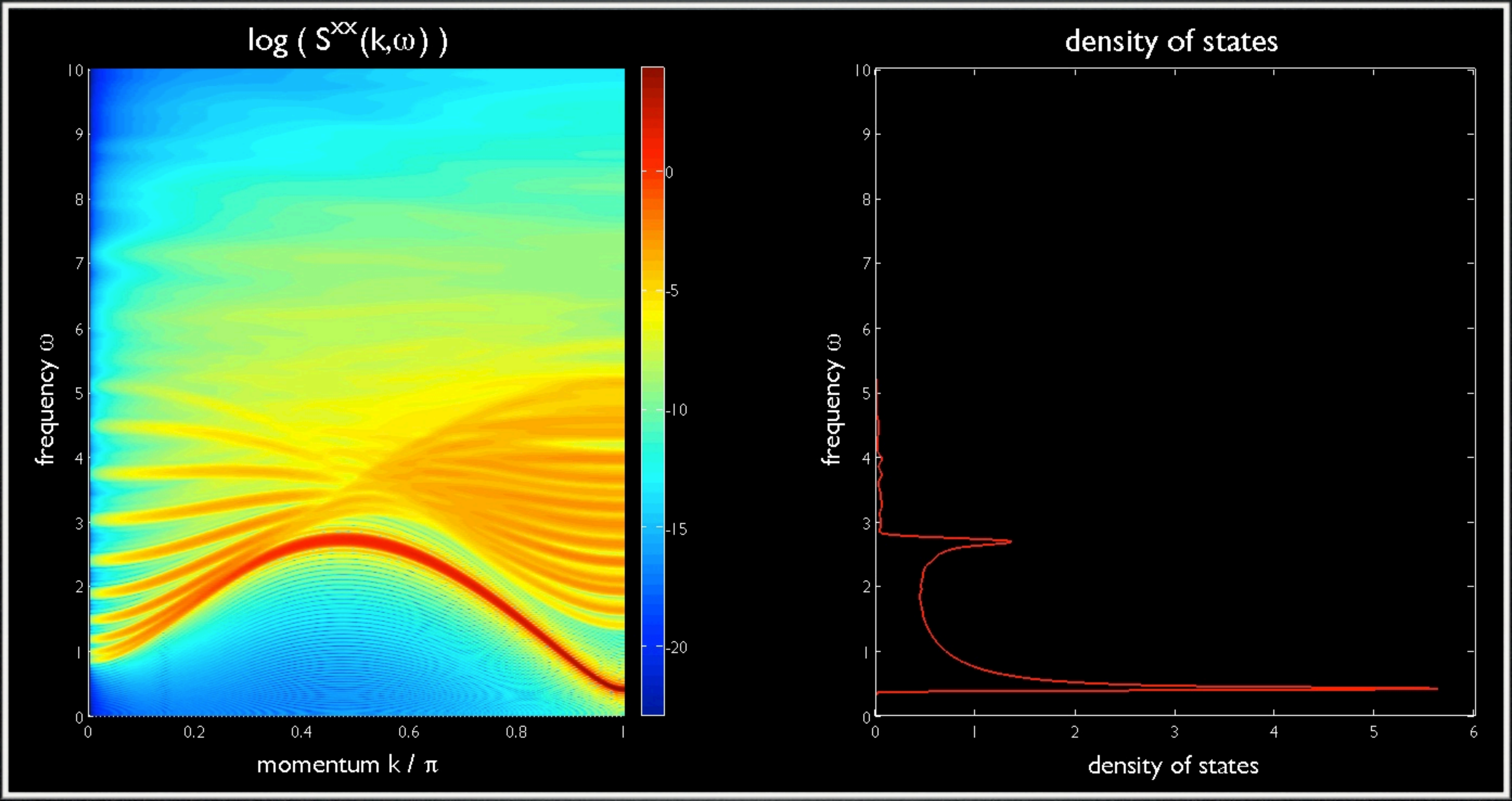
$$S^{\alpha,\beta}(k,\omega) = \langle\Psi|(\hat{O}_k^{\alpha})^{\dagger}\hat{P}_{\mathbb{T}}\delta(\omega-\hat{H})\hat{P}_{\mathbb{T}}\hat{O}_k^{\beta}|\Psi\rangle$$

$$\approx \langle\Psi|(\hat{O}_k^{\alpha})^{\dagger}\delta\underbrace{(\omega-\hat{P}_{\mathbb{T}}\hat{H}\hat{P}_{\mathbb{T}})}\hat{O}_k^{\beta}|\Psi\rangle$$

efficient implementation: Chebyshev decomposition

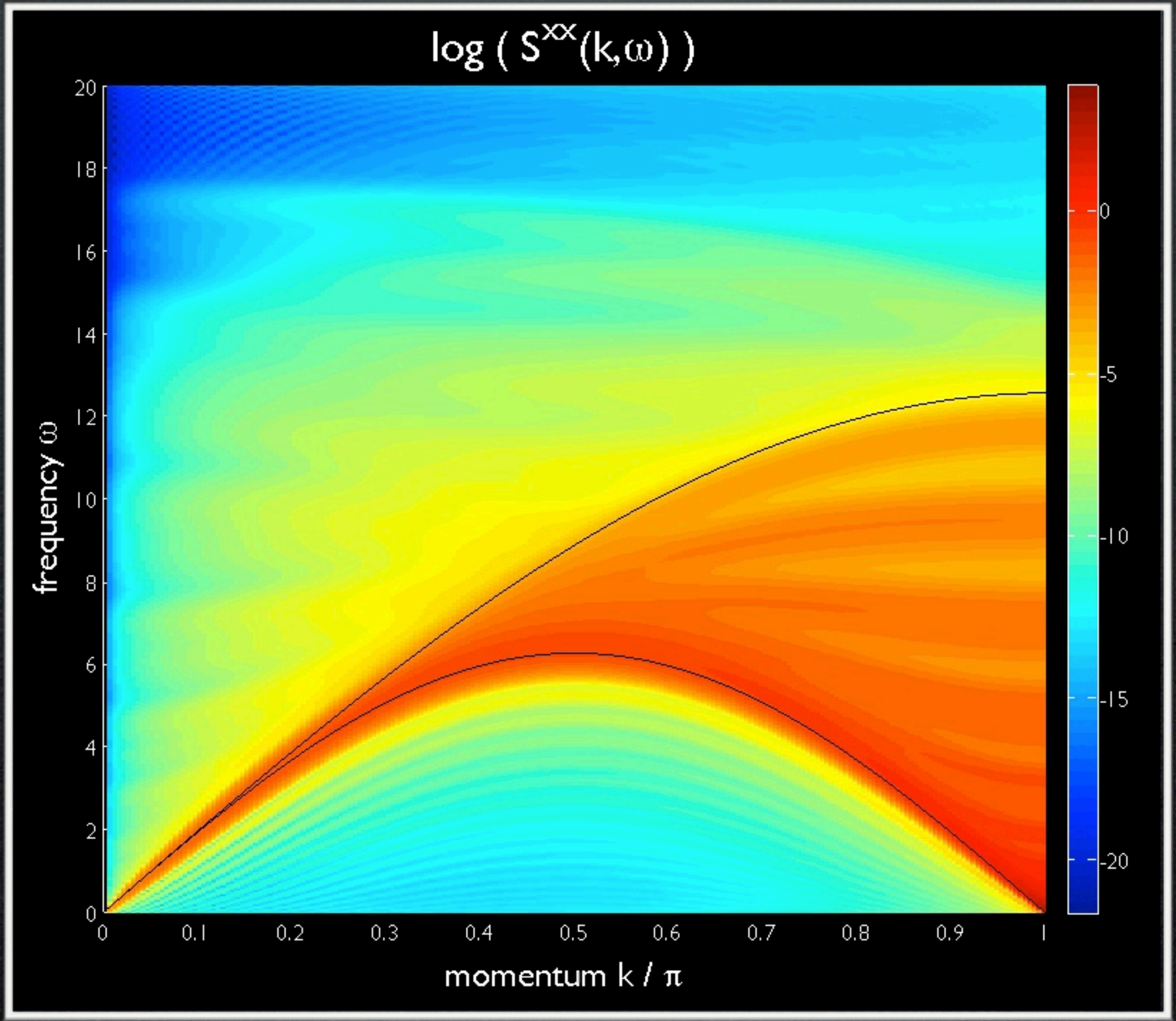
Spectral functions: some preliminary results

S=1 Heisenberg AFM: (D=192, $N_{chebychev}$=500)



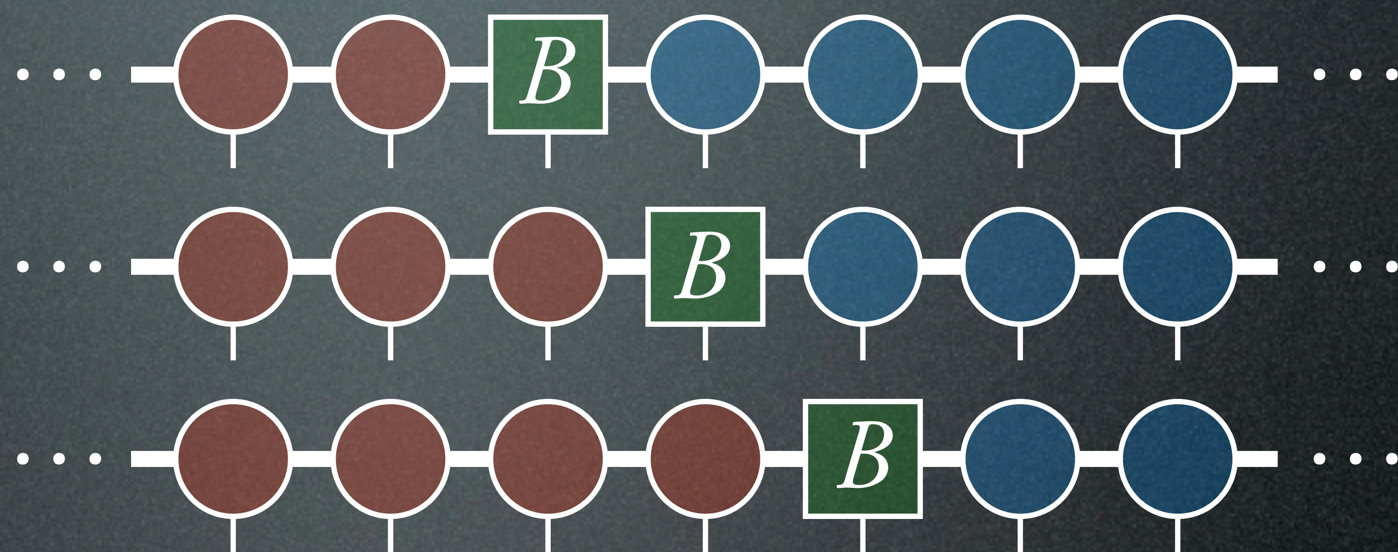
Spectral functions: some preliminary results

S=1/2 Heisenberg AFM: (D=256, $N_{chebychev}$=100)



Generalization I: domain walls

$$|\Xi(B)\rangle = \mathrm{e}^{ik(n-1)} \quad + \mathrm{e}^{ikn} \quad + \mathrm{e}^{ik(n+1)} \quad + \ldots$$

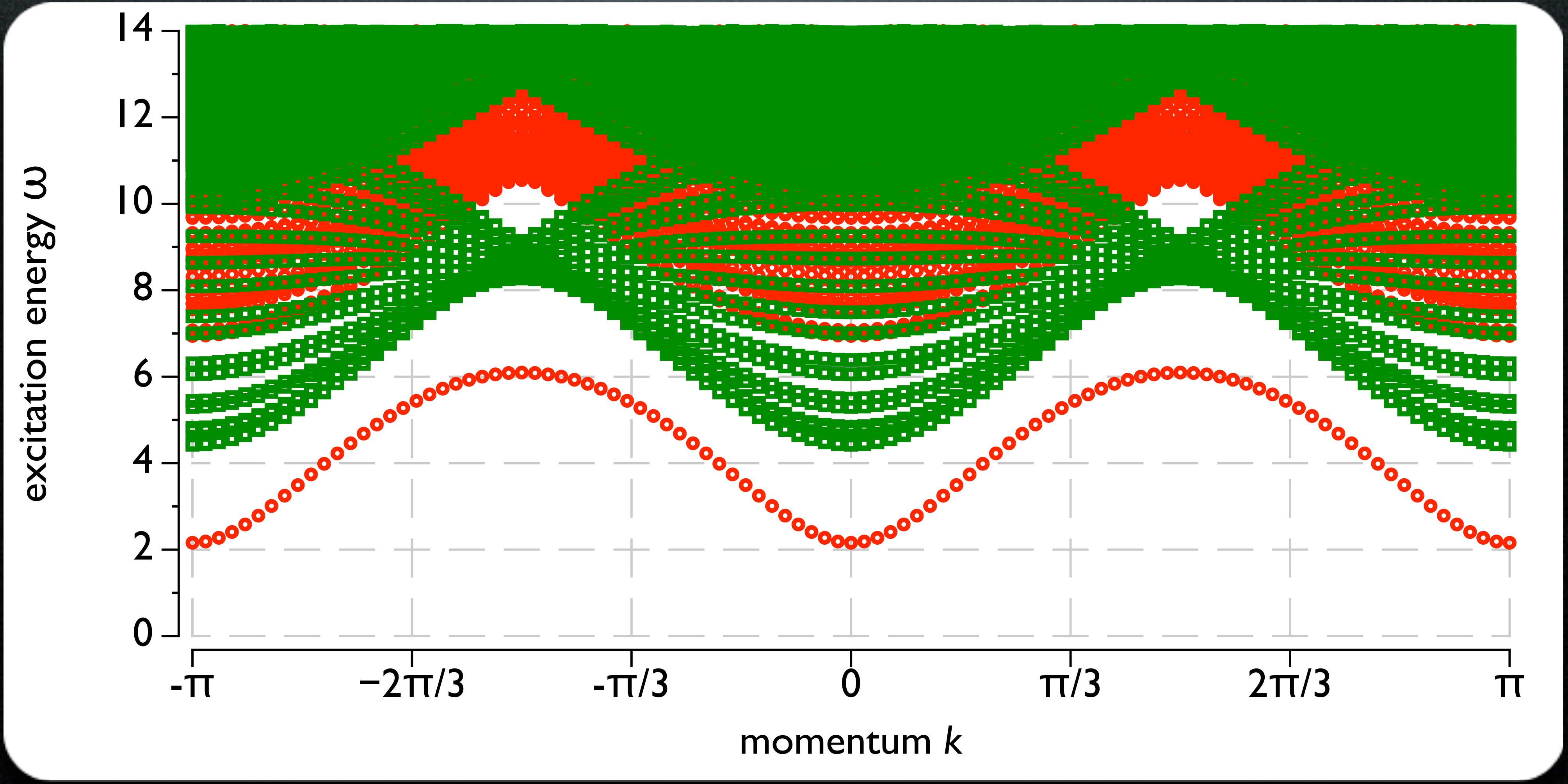


⇒ Ansatz for domain-walls with momentum k

Contains:
- Mandelstam ansatz

Generalization I: domain walls

XXZ model: $\hat{H} = \sum_{n\in\mathbb{Z}} \hat{\sigma}^x_n \hat{\sigma}^x_{n+1} + \hat{\sigma}^y_n \hat{\sigma}^y_{n+1} + \Delta \hat{\sigma}^z_n \hat{\sigma}^z_{n+1}$



Generalization I: domain walls

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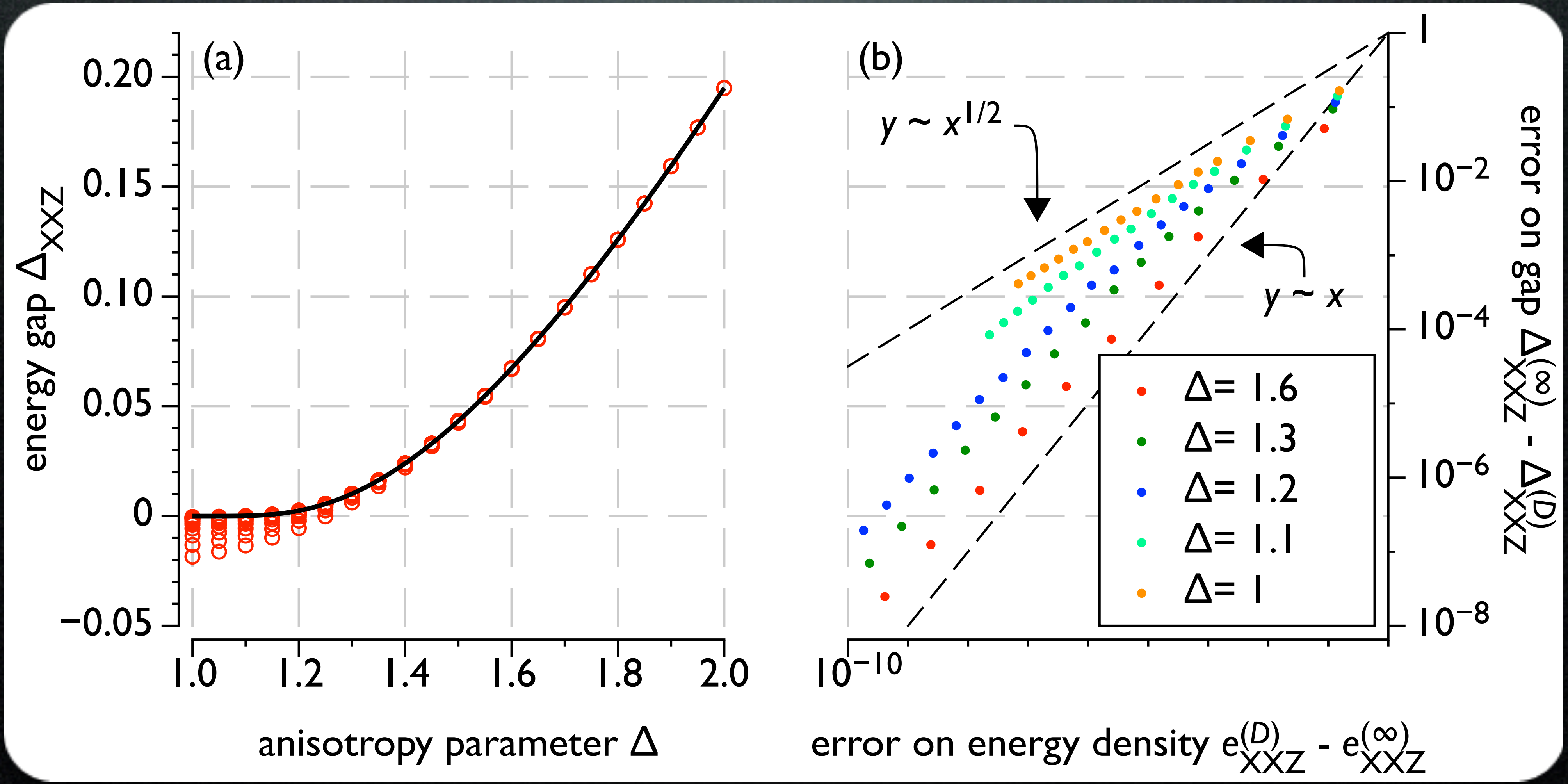
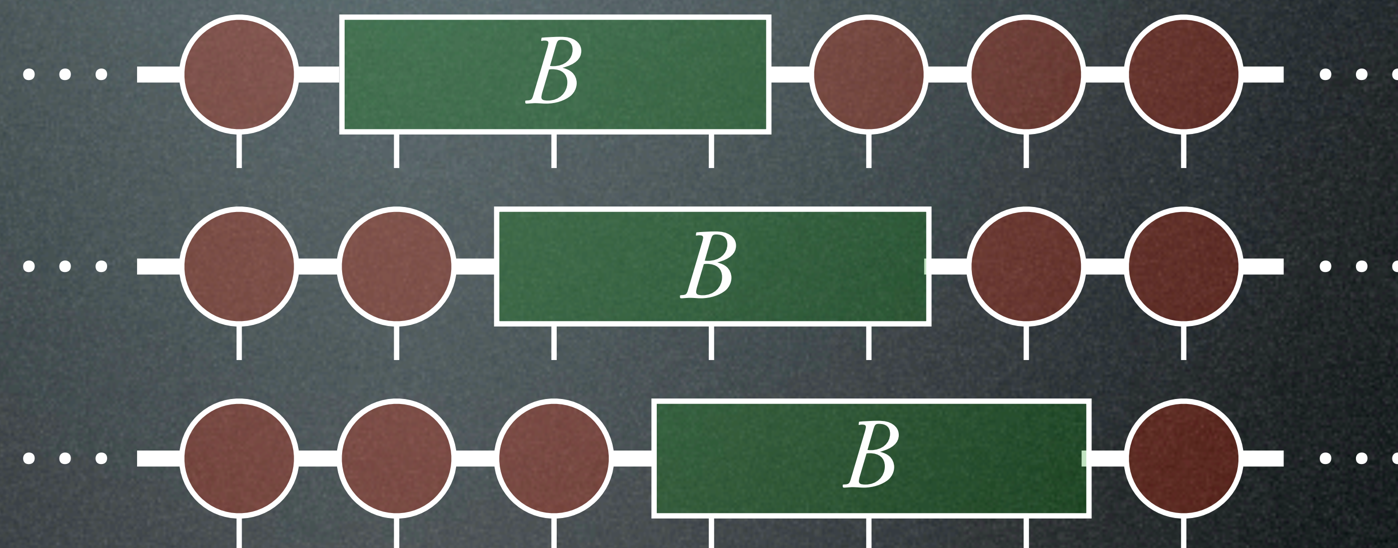


Generalization II: extended excitations

$$|\Phi(B)\rangle = e^{ik(n-1)} \quad + e^{ikn} \quad + e^{ik(n+1)} \quad + \dots$$



Exact diagonalization

MPS decomposition

Generalization II: extended excitations

AKLT model:

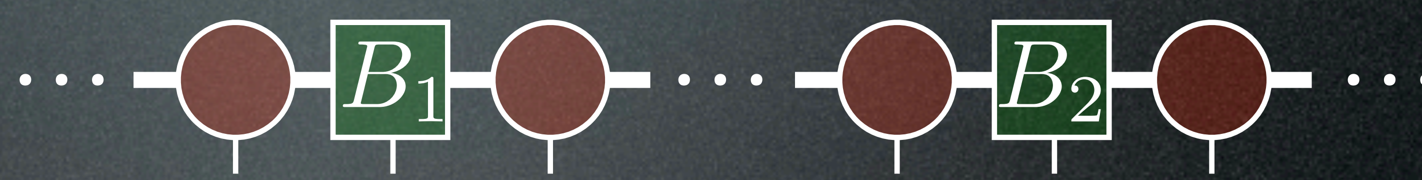
number of sites	gap
1	0.740740740740
2	0.701269162172
3	0.70033040443
4	0.70025834615
5	0.70024953788
6	0.70024845087

Generalization III: 2-particle excitations

$$|\partial_i \partial_j \Psi(A)\rangle$$

$$\Downarrow$$

$$\sum_{n_1 \neq n_2} \mathrm{e}^{\mathrm{i}k_1 n_1 + \mathrm{i}k_2 n_2}$$



- Improve spectral functions?
- Study particle scattering?

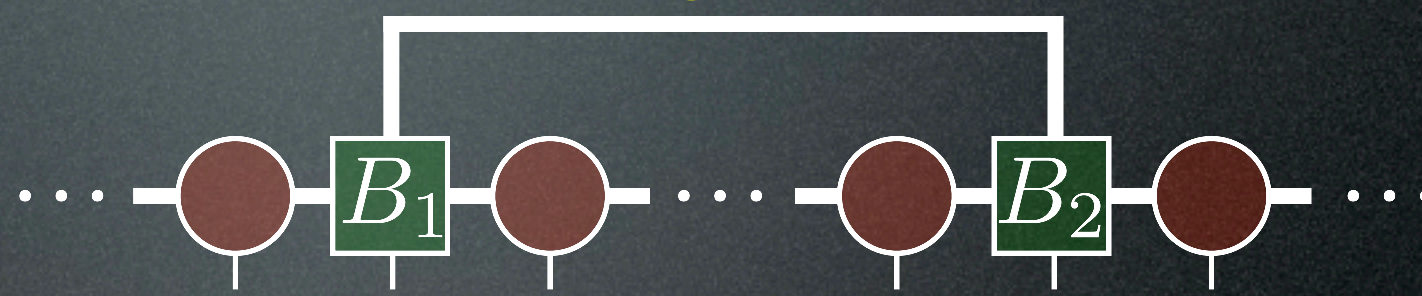
Generalization III: 2-particle excitations

$$|\partial_i \partial_j \Psi(A)\rangle$$

$$\Downarrow$$

$$\sum_{n_1 \neq n_2} \mathrm{e}^{\mathrm{i}k_1 n_1 + \mathrm{i}k_2 n_2}$$

particle entanglement



- Improve spectral functions?
- Study particle scattering?

Generalization IV: Fock space construction

$\Rightarrow$ Generalization to any finite number of particles

$\downarrow$

Fock space construction on a non-trivial vacuum provided by the MPS ground state

Conclusions:

- Systematic framework for time evolution, excitations, spectral functions, ... by exploiting the MPS **geometry (tangent plane)**
- Efficient implementation possible!
- Symmetry inherently respected
- Very flexible idea: much room for generalizations and extensions

$\rightarrow$ What about PEPS, MERA, ... ?

Thank you!

Questions?