Entanglement and variational methods for strongly correlated quantum many-body systems

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Outline

- The variational method in quantum many-body systems
- Guiding principle: area law for entanglement entropy
- Variational classes for gapped phases:
  - Matrix product states for 1+1 D quantum spin systems
  - Projected entangled pair states for 2+1 D systems
  - Continuous MPS for quantum field theories

Why do we need a variational principle?

1. Central goal in quantum mechanics (particle physics, condensed matter, quantum chemsitry, …) is to describe the low-energy (long-range) physics of (effective) Hamiltonians

   – Quantum features most prevalent at low temperature
   – For most fermionic systems, room temperature is already very cold (Fermi T = 10.000 K)

2. The size of the Hilbert space associated to a many-body quantum system scales exponentially in the number of particles/spins/…

   – We have to resort to approximate methods to describe generic quantum many-body systems
   – Physical states are very far from being random: they have nontrivial local properties!
   – Hilbert space is a convenient illusion (Qarry, FV PRL ‘11)

Why do we need a variational principle?

3. Several of the biggest breakthroughs in quantum many-body physics involved the variational principle:

   - Helium atom (Hylleraas, …)
   - Hartree-Fock for quantum chemistry
     - Also starting point for conventional QFT
   - BCS theory for superconductivity
   - Laughlin wavefunctions for fractional quantum Hall effect
   - DMRG of S. White for quantum spin systems

4. The variational principle allows to capture non-perturbative effects very effectively

The variational method

- Basic principle: given a Hamiltonian H, we would like to identify the ground state (and more general all low energy states). Instead of working in the full Hilbert space, we want to find the states with minimal energy that live in some manifold parameterized by the parameters x.
  - Note: the whole trick is to identify the right manifold!

- Ritz variational principle:

$$E_0(H) \leq \min_x \frac{\langle \psi(x)|H|\psi(x)\rangle}{\langle \psi(x)|\psi(x)\rangle}$$

- If the system has a gap and the variational wavefunction has an energy smaller than the first excited state, then the variational wavefunction has a sizeable overlap with the true ground state

- Obviously, the whole trick is to identify the right class of wavefunctions for the problem at hand
  - ***What are the guiding principles?***

- In many very relevant cases, slight variations/perturbations on Gaussian states work extremely well:
  - For quantum chemistry, state of the art is the coupled cluster method (refinement of Hartree-Fock theory)
  - BEC: Gaussian, Gross-Pitaevakii, …
  - For quantum field theory in the small coupling regime: perturbation theory (Feynman diagrams) on top of Gaussians

- However, many exotic materials do not fall within this class: quantum Hall systems, strongly correlated electrons on a lattice (Hubbard model), …
  - Those systems exhibit nontrivial *entanglement*

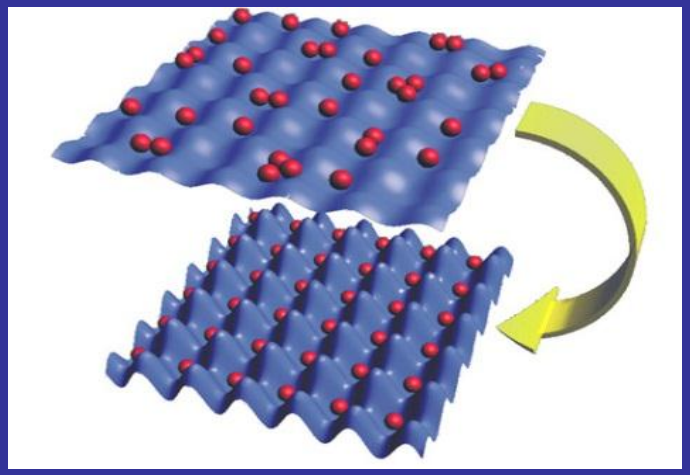
Entanglement

- From point of view of quantum information theory, it is a resource
  - Quantification: how useful is a quantum state/system to do information theoretic tasks
    - E.g. atomic clocks, quantum communication, quantum computing
- From the point of view of numerical simulation strongly correlated quantum systems, quantum chemistry: enemy nr. 1 !
- From the point of view of condensed matter and high energy physics: leads to great things like quantum phase transitions, topological quantum order, …
- Key question: what kind of superpositions appear in nature ?

Quantum spin systems

- Playground for strongly interacting many-body systems

- Have been of intense interest since Heisenberg and Bethe since the '30s because of the fact that they provide effective models for describing magnetism, quantum phase transitions, …
  - More recently: huge surge of interest due to optical lattice experiments

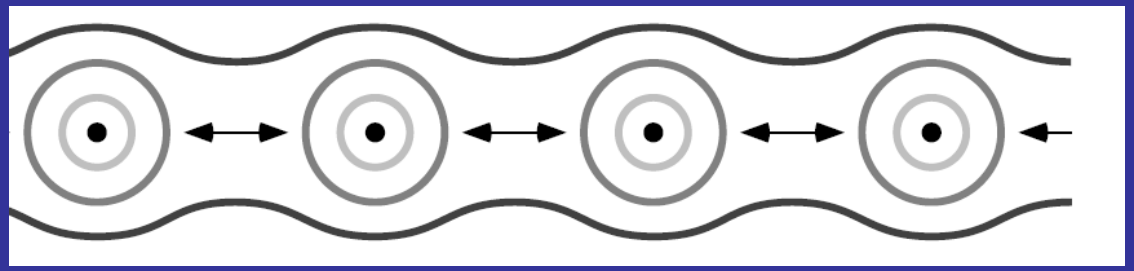


- Simplest model: the Hubbard model

$$H = H_{\text{hop}} + H_{\text{int}}.$$

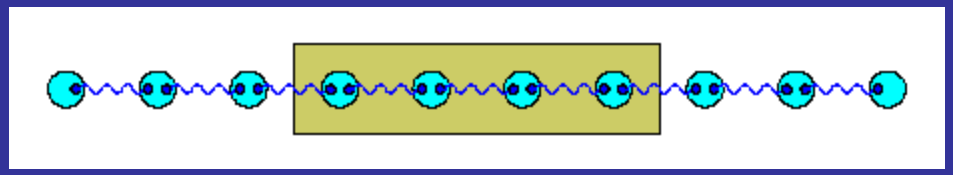
$$H_{\text{hop}} = \sum_{x,y\in\Lambda} \sum_{\sigma=\uparrow,\downarrow} t_{x,y}\, c^{\dagger}_{x,\sigma} c_{y,\sigma}$$

$$H_{\text{int}} = \sum_{x\in\Lambda} U_x\, n_{x,\uparrow} n_{x,\downarrow}$$



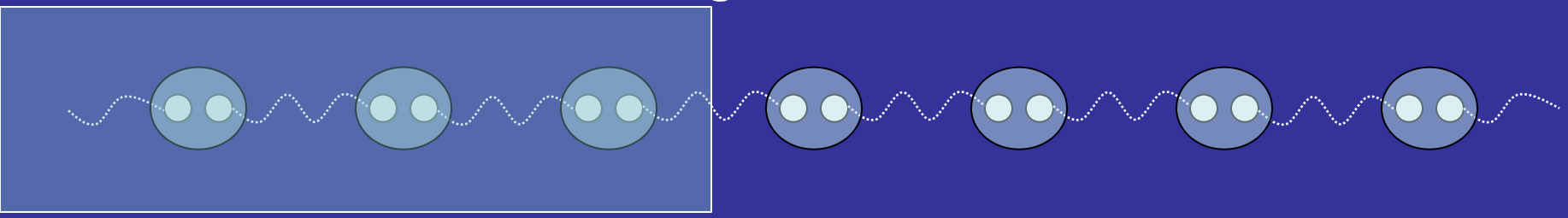
Area law for entanglement entropy

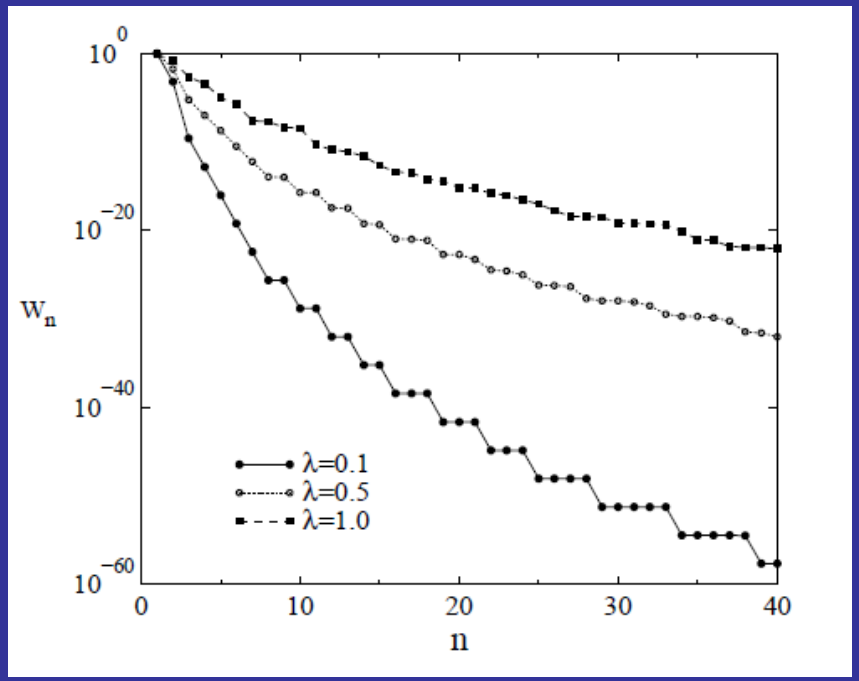
- All low-energy states of local Hamiltonians on the lattice exhibit very few entanglement (area law)



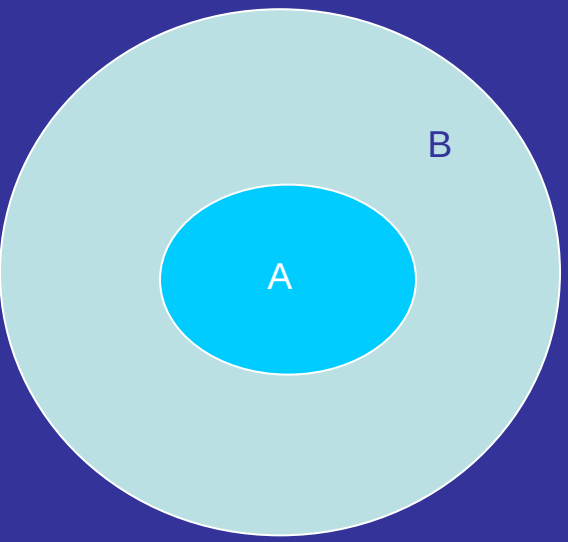
- This is a guiding principle: we will create a new class of variational wavefunctions (tensor networks) that parameterizes all states with that property

Schmidt coefficients for Ising model in transverse magnetic field:





Area laws for thermal states of local Hamiltonians



Quantifying the amount of correlations between A and B: mutual information

$$I_{AB} = S(\rho_A) + S(\rho_B) - S(\rho_{AB})$$

All thermal states exhibit an exact area law (as contrasted to volume law)

$$\rho_{AB} \approx \exp(-\beta H)$$

$$F(\rho_A \otimes \rho_B) = Tr(H\rho_A \otimes \rho_B) - \frac{S(\rho_A \otimes \rho_B)}{\beta} \geq Tr(H\rho_{AB}) - \frac{S(\rho_{AB})}{\beta}$$

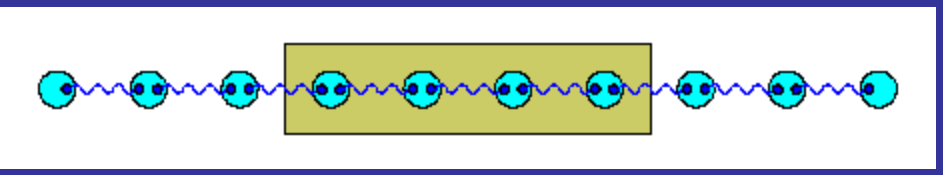
$$\Rightarrow I_{AB} \leq \beta\, Tr(H[\rho_A \otimes \rho_B - \rho_{AB}]) = \beta\, Tr(H_{AB}[\rho_A \otimes \rho_B - \rho_{AB}])$$

Cirac, Hastings, Wolf, FV. PRL‘08

- All correlations are *localized* around the boundary

Area laws

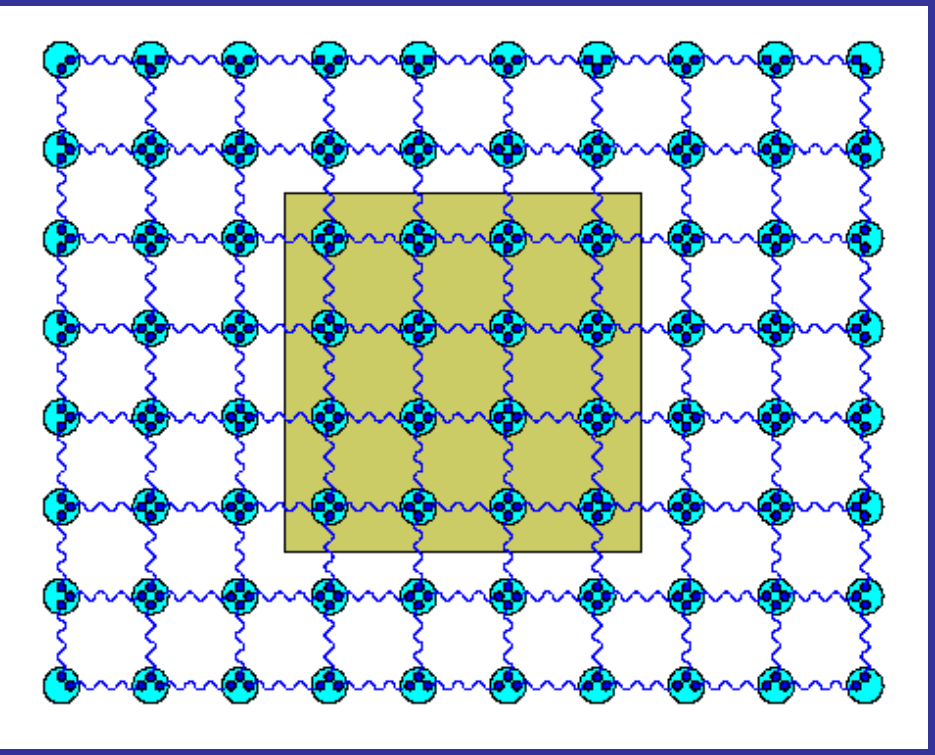
- Ground states have extremal local correlations compatible with e.g. translation symmetry; this gives rise to correlation lengths, and entanglement is shared between particles within this correlation length. Therefore, the entanglement of a block with the outside scales as the surface area and not as the volume of the block
- Main picture: entanglement / information is concentrated around the boundary



$$\text{Gapped}: \quad S\left(\rho_{1,2,\cdots,L}\right) \approx \frac{c+\bar{c}}{6}\ln\left(\xi\right)+\ldots$$

$$\text{Critical}: \quad S\left(\rho_{1,2,\cdots,L}\right) \approx \frac{c+\bar{c}}{6}\ln\left(L\right)+\ldots$$

Vidal, Kitaev, Cardy, Korepin



$$\text{Gapped}: \quad S\left(\rho_{1,2,\cdots,L^2}\right) \approx a.\mathrm{L}+\cdots$$

$$\text{Critical}:$$

$$\text{Free fermions}: \quad S\left(\rho_{1,2,\cdots,L^2}\right) \approx a.L\ln L+\ldots$$

$$\text{Critical spin}: \quad S\left(\rho_{1,2,\cdots,L^2}\right) \approx a.L+\ldots$$

Wolf, Klich

Topological entropy: detects topological quantum order locally!

$$S\left(\rho_{ABC}\right)-S\left(\rho_{AB}\right)-S\left(\rho_{AC}\right)-S\left(\rho_{BC}\right)+S\left(\rho_{A}\right)+S\left(\rho_{B}\right)+S\left(\rho_{C}\right)$$

Kitaev, Preskill, Levin, Wen

New guiding principle for interacting systems on the lattice: area law for entanglement entropy

- The corner in Hilbert space containing such low-energy states can be fully parameterized by tensor network states : the entanglement is distributed in a *local* way such as to capture the area law in a way that does not lead to an exponential number of parameters

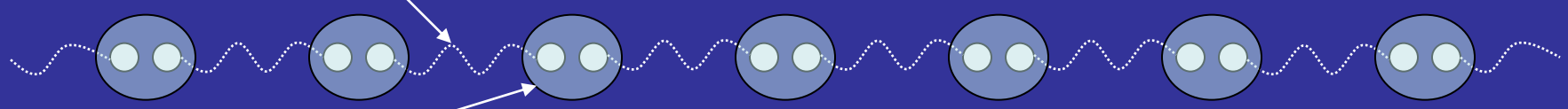
    - Matrix product states (MPS) in 1D
    - projected entangled pair states (PEPS) in higher dimensions
    - multiscale entanglement renormalization ansatz for critical systems (Vidal)

In fact, for gapped 1-dimensional quantum spin systems, we can understand all physics by looking at matrix product states; this allows e.g. for a classification of all possible phases of 1-D systems using MPS formalism
Same in principle for higher dimensional classifications using PEPS

Tensor network states

- 1D case: Matrix product states, which are generalizations of the valence bond AKLT-states of Affleck-Kennedy-Lieb-Tasaki ('88)

$$|I\rangle = \sum_{i=1}^{D} |i\rangle |i\rangle$$



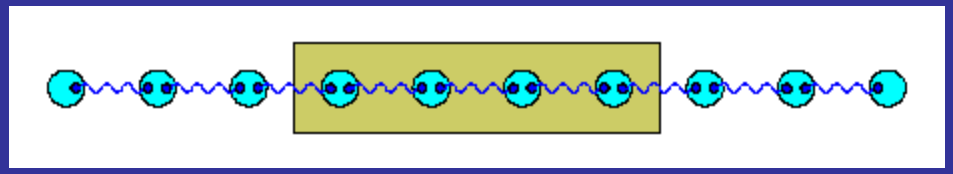
$$\text{Map A}: H^D \otimes H^D \to H^d$$

- Systematic way of constructing translational invariant states
- "Virtual" dimension D encodes the "renormalized" degrees of freedom of the environment

- Inherently used by Wilson (NRG) and S. White (DMRG): NRG and DMRG are variational methods within the class of MPS

Matrix product states and area laws

- All MPS exhibit very few block entanglement : $S_\alpha(\rho_{1..L}) \le 2\log D$



$$S_\alpha(\rho) = \frac{\log Tr\rho^\alpha}{1-\alpha} \; ; 0 \le \alpha$$

- Converse is also true: if the block entropy is measured by Renyi entropies with $0 \le \alpha < 1$, then small entanglement implies approximable by MPS

$S_\alpha \sim$	const	$\log L$	$L^\kappa (\kappa<1)$	L
$S_{\alpha<1}$	approximable		undetermined	
$S \equiv S_1$	undetermined			
$S_{\alpha>1}$	undetermined		inapproximable	

suppose $\forall L, N : S_\alpha(\rho^N_{1..L}) \le c \log L$

then $\forall \varepsilon, N; \exists D \le \frac{1}{\varepsilon} N^{f(c)}$:

$$\left\| \left|\psi^N_{ex}\right\rangle - \left|\psi^N_D\right\rangle \right\| \le \varepsilon$$

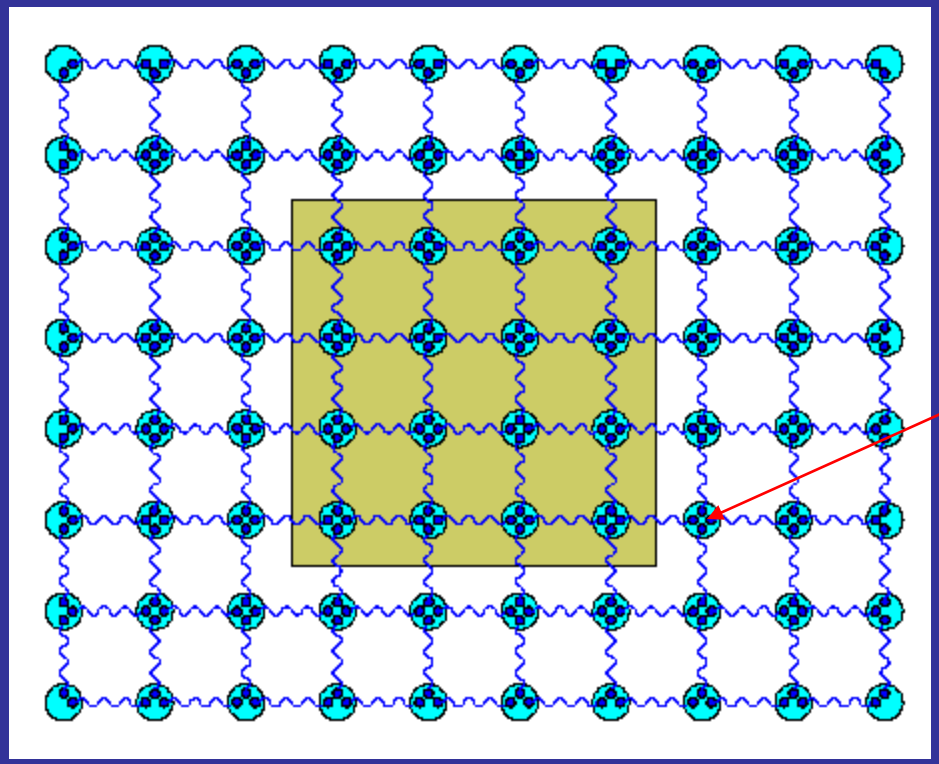
Note: log(L) behaviour saturated for critical systems in 1D

Cfr. Peshel, Vidal, Cardy, Korepin, Cardy, Calabrese …

FV, Cirac , Schuch “06; Hastings ‘08

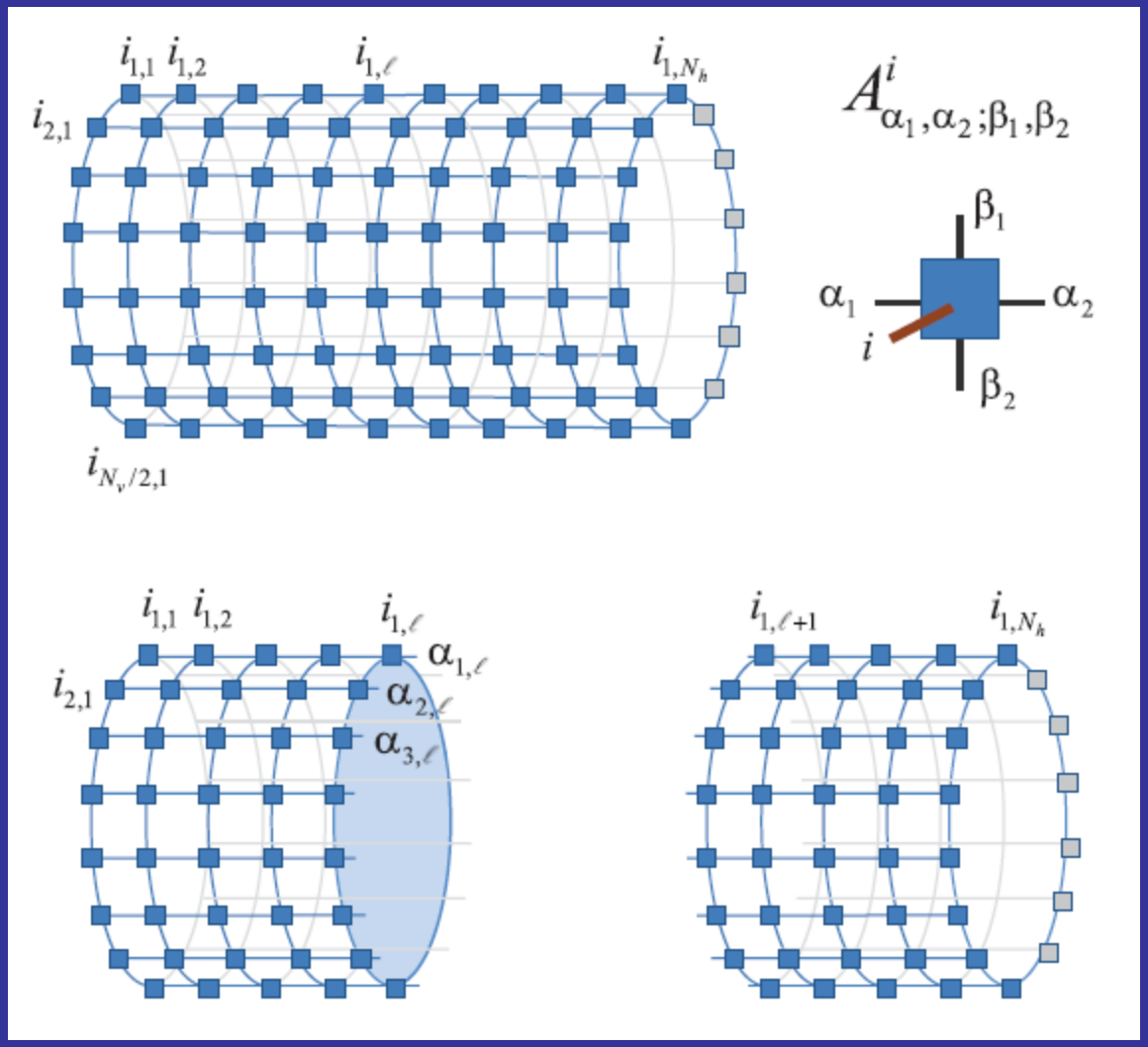
Tensor networks in 2D: PEPS

FV, Cirac '04



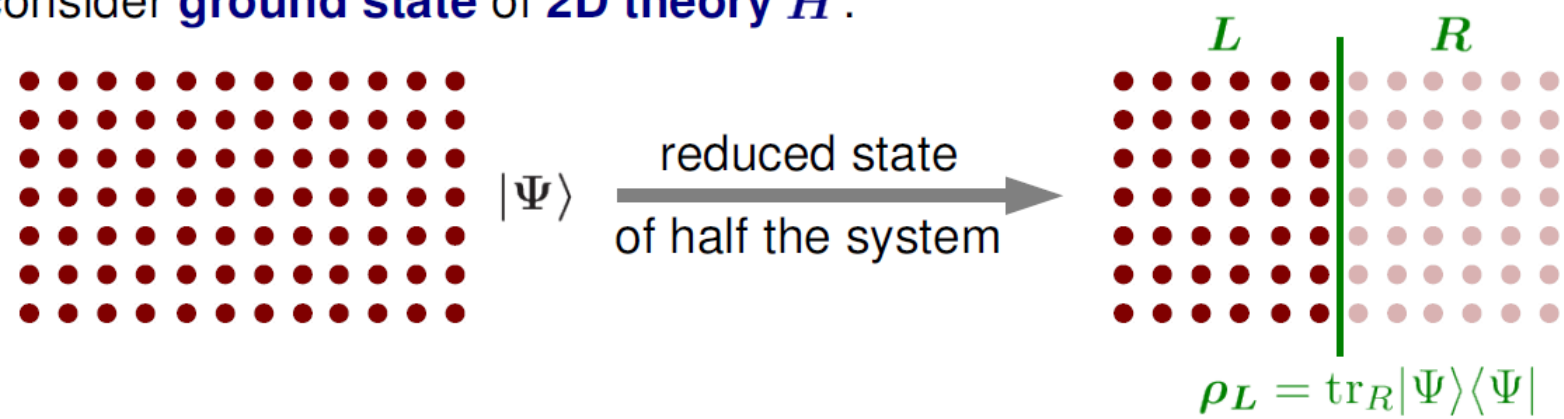
Tensor P maps D^4 dimensional to d dimenional space

- Conjecture: any ground state of a local gapped Hamiltonian can be written efficiently within this form (# parameters is D^4)
- In this case, the correlation length can diverge
- Examples of exotic PEPS: AKLT, RVB, Kitaev's toric code, Levin-Wen models, …
  - The order parameters and/or topological features are reflected in the ***local*** symmetry properties of the tensors!


$i_{1,1}$ $i_{1,2}$ $i_{1,\ell}$ i_{1,N_h}
$i_{2,1}$
$i_{N_v/2,1}$
$A^{i}_{\alpha_1,\alpha_2;\beta_1,\beta_2}$
β_1
α_1
α_2
i
β_2
$i_{1,1}$ $i_{1,2}$ $i_{1,\ell}$
$\alpha_{1,\ell}$
$i_{2,1}$
$\alpha_{2,\ell}$
$\alpha_{3,\ell}$
$i_{1,\ell+1}$ i_{1,N_h}

Entanglement spectrum and boundary theories

- consider **ground state** of **2D theory** H :



- $\mathrm{spec}(\rho_L)$: **"entanglement spectrum"** of system
- observation: $\log(\mathrm{spec}(\rho_L))$ corresponds to **spectrum of 1D theory**!

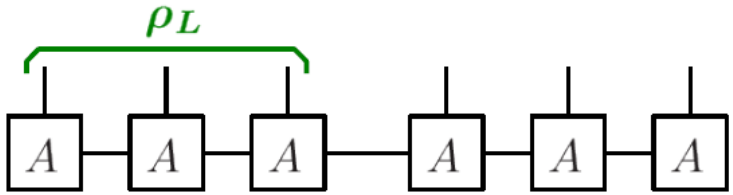
$\rightarrow$ **"boundary theory"** H_{bnd}

- Dimension mismatch: ρ_L is two-dimensional, H_{bnd} is one-dimensional!

Is there a natural way to obtain a one-dimensional boundary model from a two-dimensional bulk theory?

Bulk-boundary mapping using PEPS

- **illustration** of idea in **one dimension**:

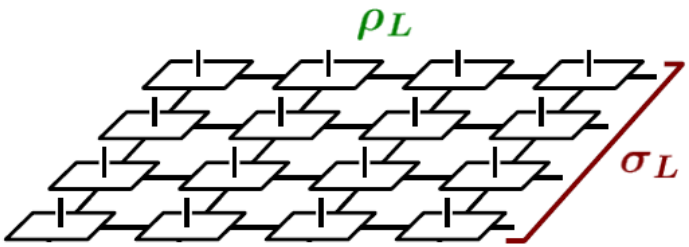


$$\rho_L = V\sqrt{\sigma_L^T}\sigma_R\sqrt{\sigma_L^T}V^\dagger$$

with symmetries:

$$\boxed{\rho = V\sigma^2 V^\dagger}$$

- analogously in **two dimensions**:



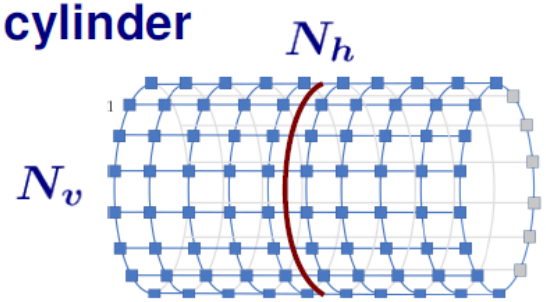
- **1D stucture** of σ emerges **naturally**
- 1D **boundary theory** H_{bnd} via

$$\sigma = \exp\left[-H_{\mathrm{bnd}}\right]$$

- isometry V establishes a **full bulk-boundary duality**

Numerical study of boundaries with PEPS

- We study models on a **cylinder**



- **interaction range** of Hamiltonian

terms with interaction range k

$$H = h_0 + h_1 + h_2 + \cdots + h_k + \ldots$$

$d_k = \mathrm{tr}[h_k^2]/2^{N_v}$: total strength of range- k terms

- **"effective temperature"** $\beta_{\mathrm{eff}} \propto \sqrt{d_2/d_0}$ (if $d_1 = 0$)

- numerical methods:
  - **column-wise** transfer operator $\rightarrow N_h = \infty$ possible
  - **arbitrary** N_v possible, but limited if we want to compute $H = \log \sigma$

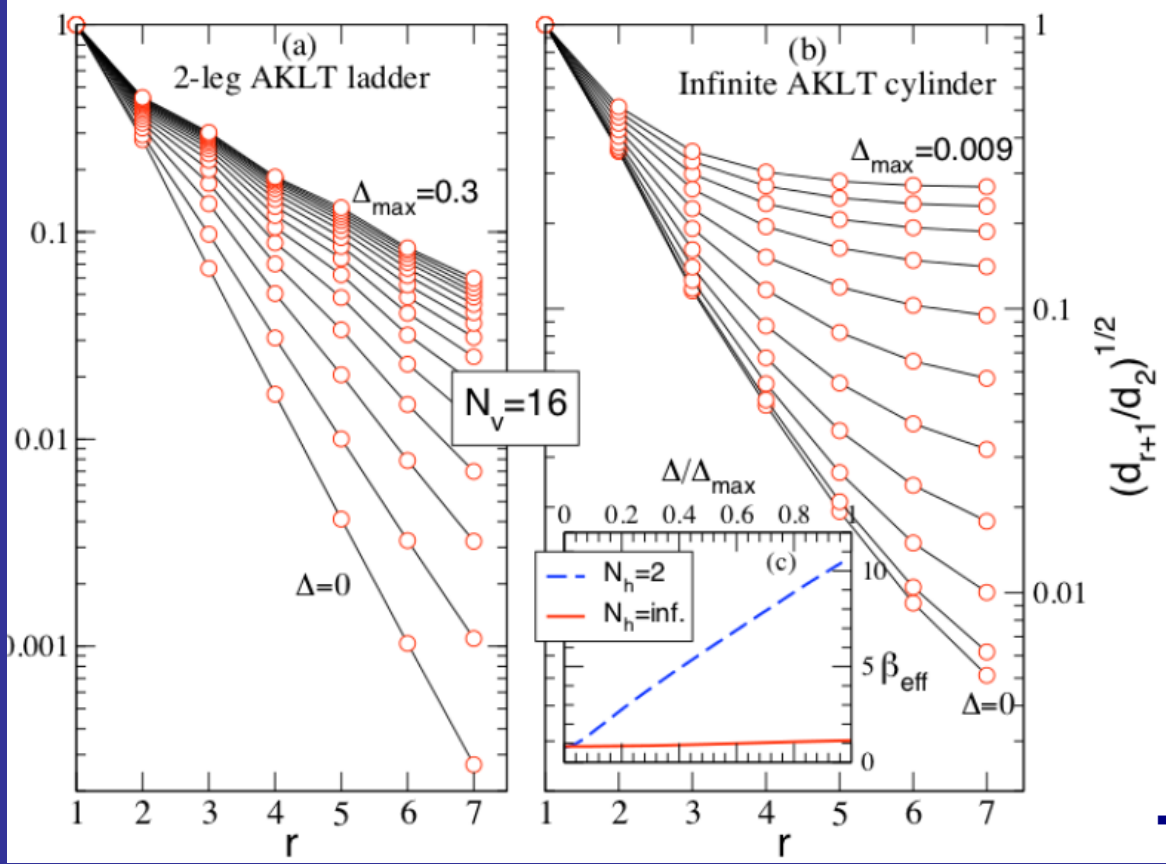
- conversely: boundary theory short-range correlated
  $\rightarrow$ efficient contraction of PEPS possible

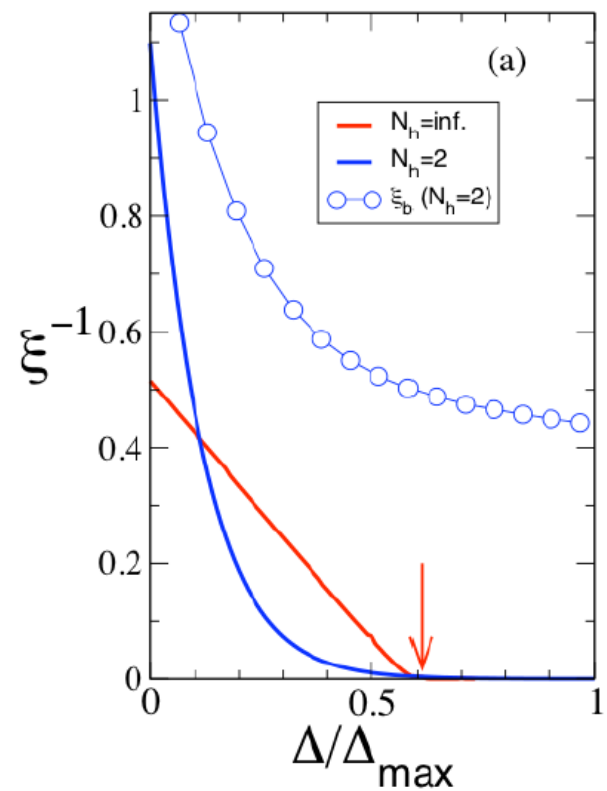
Deformed AKLT model

- 2D square lattice **AKLT model** ($S = 2$) with "nematic field"

$$H = \sum_{<i,j>} Q_i(\Delta) Q_j(\Delta) P_{i,j}^{S=4} Q_i(\Delta) Q_j(\Delta) \qquad Q_i(\Delta) = e^{-8\Delta S_{z,i}^2}$$

- has exact PEPS ground state $(Q(\Delta)^{-1})^{\otimes N} |\Psi_{\mathrm{AKLT}}\rangle$





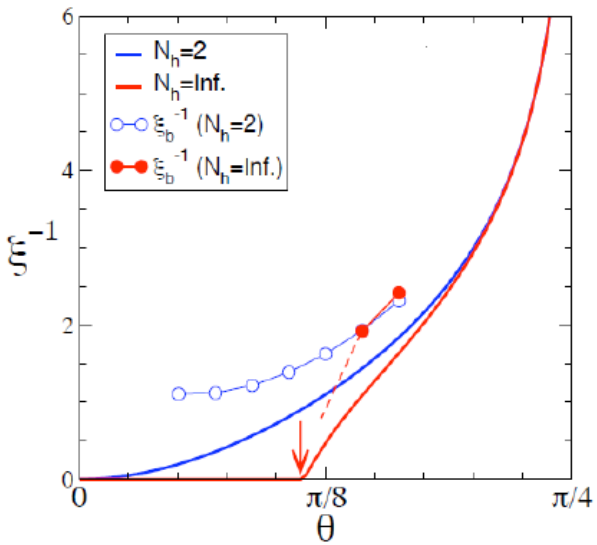
Criticality and the boundary model

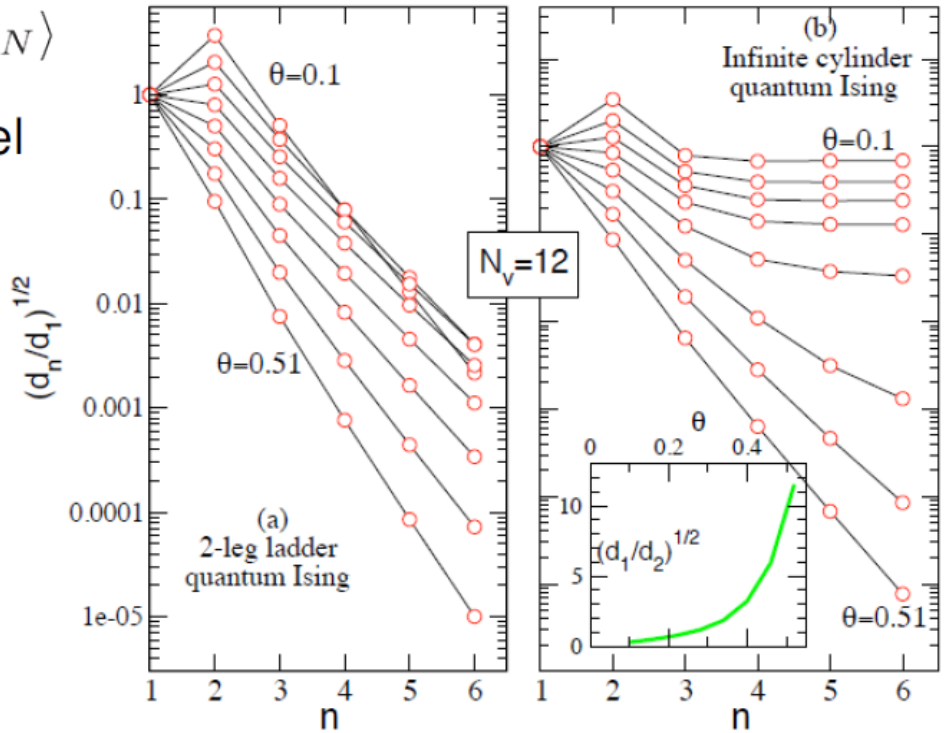
- **ladders**: divergent correlations caused by **effective temperature** going to zero
- **2D systems**: diverging correlations at phase transition arise from **diverging interaction length** at **finite effective temperature**

- confirmed with **Ising PEPS**:

$$|\psi_\beta\rangle = \sum e^{-\beta H(s_1,\ldots,s_N)/2}|s_1,\ldots,s_N\rangle$$

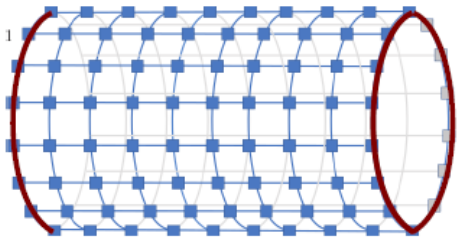
with $H(s_1,\ldots,s_N)$ 2D Ising model





Boundary theory for topological models

- What about the boundary theory of **topological models**?



- **Kitaev's toric code**: left and right **boundaries are connected**

$$\sigma_{LR} = \mathbb{1}^{\otimes N_v} \otimes \mathbb{1}^{\otimes N_v} + X^{\otimes N_v} \otimes X^{\otimes N_v}$$

$\Rightarrow$ **boundary model** $H_{\mathrm{bnd}} = X^{\otimes N_v}$ is completely **non-local**,
eff. **temperature** depends on **other boundary**

- adding **local magnetic field** breaks connection between boundaries

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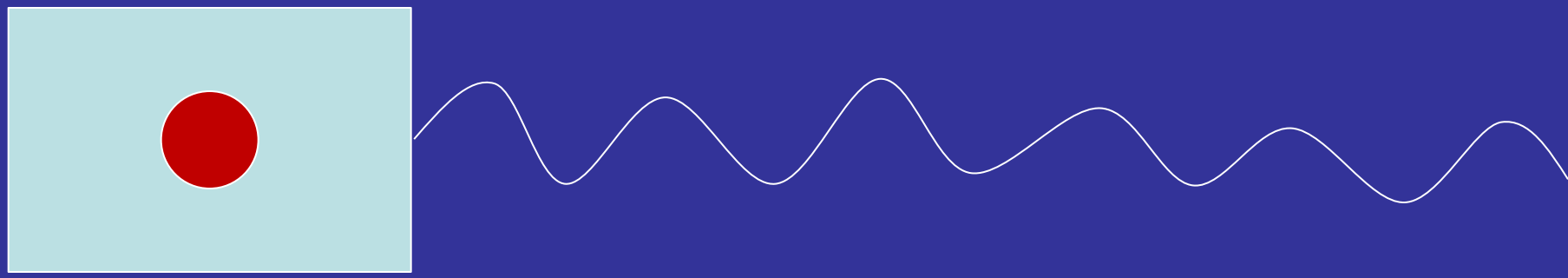
- different from Ising model:

$$\sigma_{LR} = |0\rangle\langle 0|^{\otimes N_v} \otimes |0\rangle\langle 0|^{\otimes N_v} + |1\rangle\langle 1|^{\otimes N_v} \otimes |1\rangle\langle 1|^{\otimes N_v}$$

$\Rightarrow$ single boundary is again a **local Ising model**

Physical realization of virtual degrees of freedom: Cavity QED

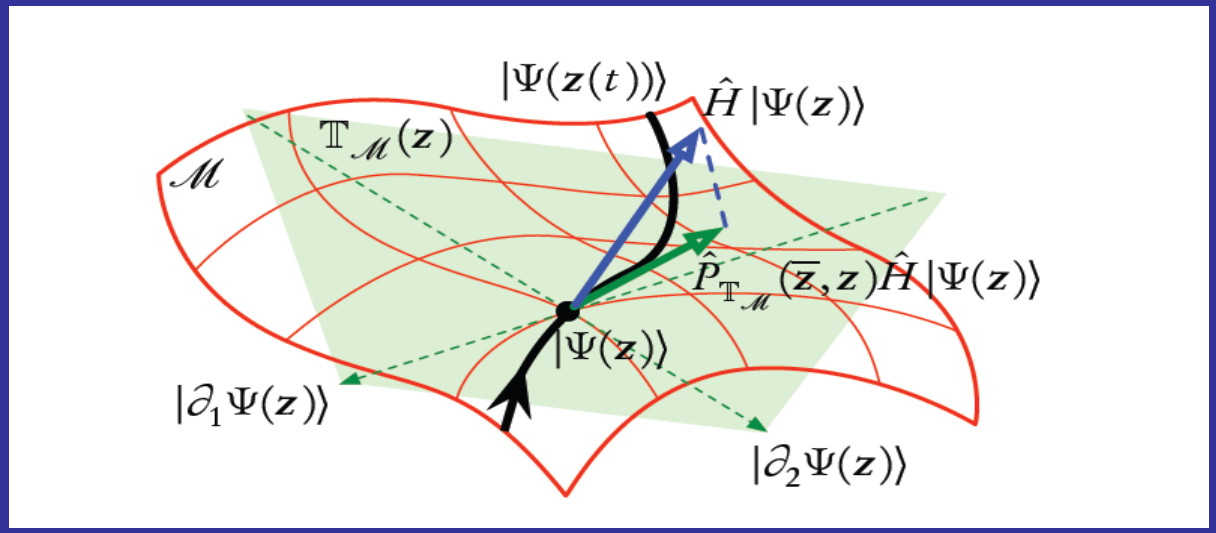


- D-level atom in the cavity
- Coupled to the cavity modes by a Hamiltonian H
- Photons leak out of the cavity
- Global quantum State of all photons leaking out of cavity is precisely described by a cMPS
- Time-time-time-… correlation functions of photons are equivalent to all correlations functions of cMPS: static properties of quantum spin systems have a counterpart as time-time correlation functions of non-equilibrium systems in a dimension lower
- Provides connection between quantum measurement theory and quantum field theory

Schon, Cirac, FV, Wolf PRL ’06;
Osborne, Eisert, FV PRL ‘10

How to optimize the tensors: The time-dependent variational principle (Dirac)

- If the true quantum states that we want to describe are well represented by states in the variational manifold, we would also like to describe the dynamics in this manifold (as a consequence of the Schrodinger equation
  - Time-dependent variational principle (e.g. time-dependent HF):



$$y = argmin_y \left\| \mathcal{H}\psi(z) - \sum_j y_j \frac{\partial\psi(z)}{\partial z_j} \right\| \quad \Rightarrow \quad i\frac{\partial z_j}{\partial t} = -y_j = f(z)$$

- A linear differential equation (Schrodinger equation) in an exponentially large Hilbert space is mapped to a nonlinear differential equation in a small dimensional manifold

example: the Gross-Pitaevskii / nonlinear Schrodinger equation

- Consider a system of bosons interacting with a point-potential (Lieb-Liniger):

$$H = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{r}_i^2} + V(\mathbf{r}_i) \right) + \sum_{i<j} \frac{4\pi\hbar^2 a_s}{m} \delta(\mathbf{r}_i - \mathbf{r}_j),$$

- We now consider the manifold of coherent states:

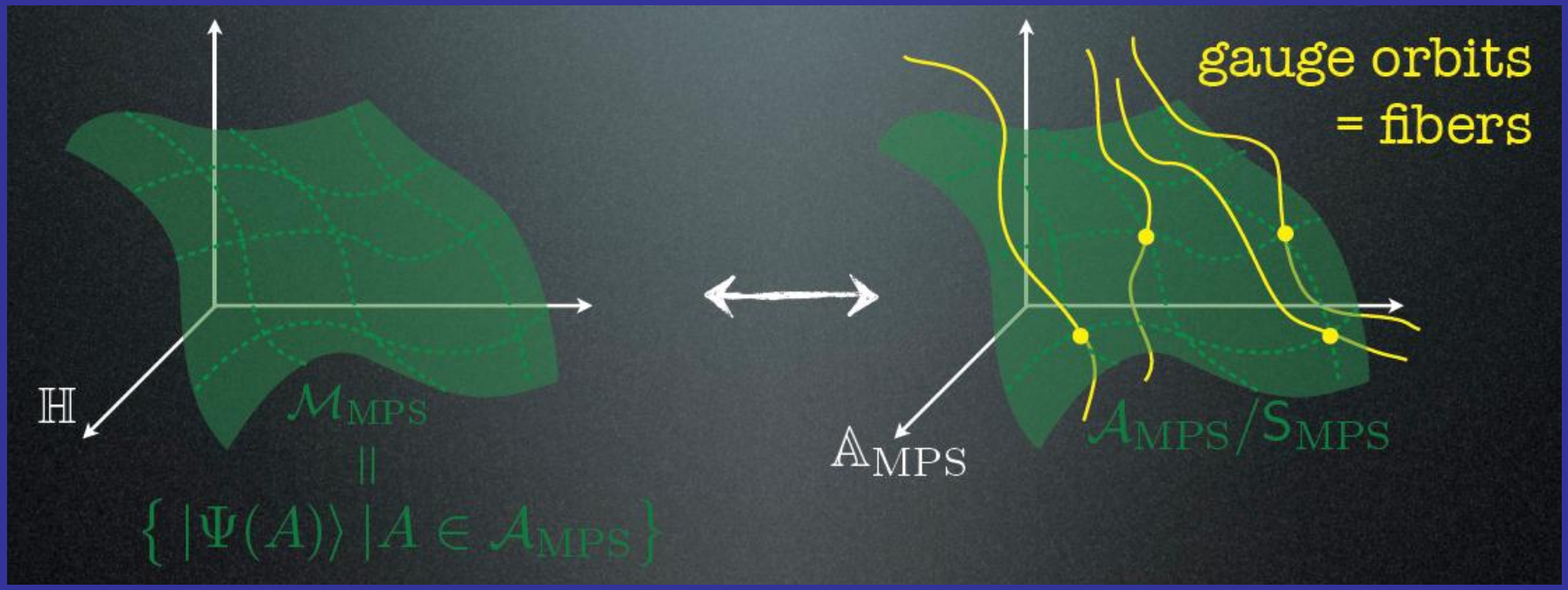
$$|\varphi\rangle = e^{\int dx\, \varphi(x) \psi_x{}^{\dagger}} |\Omega\rangle \qquad \left[\psi_x \ , \ \psi_y{}^{\dagger}\right] = \delta(x-y)$$

  – Applying the time-dependent variational principle, a straightforward calculation yields the Gross-Pitaevskii equation:

$$-i\partial_t \phi(\mathbf{x}, t) = \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{x}) \right) \phi(\mathbf{x}, t) + g|\phi(\mathbf{x}, t)|^2 \phi(\mathbf{x}, t)$$

  – Ground states can be approximated by evolving in imaginary time

Manifold of MPS: fibre bundles

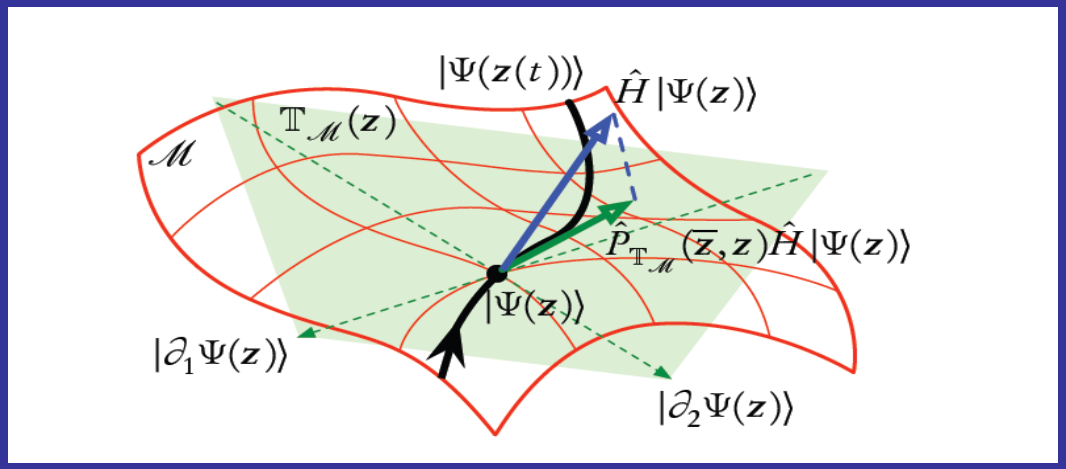


- MPS description is not unique: there are gauge degrees of freedom

$$A^i \leftrightarrow X A^i X^{-1}$$

  – Those gauge transformation play crucial role in classifying all phases of matter in 1D (Gu, Wen ‘09; Pollman et al ‘09; Schuch, Cirac ‘11; …)

Time dependent variational principle for MPS



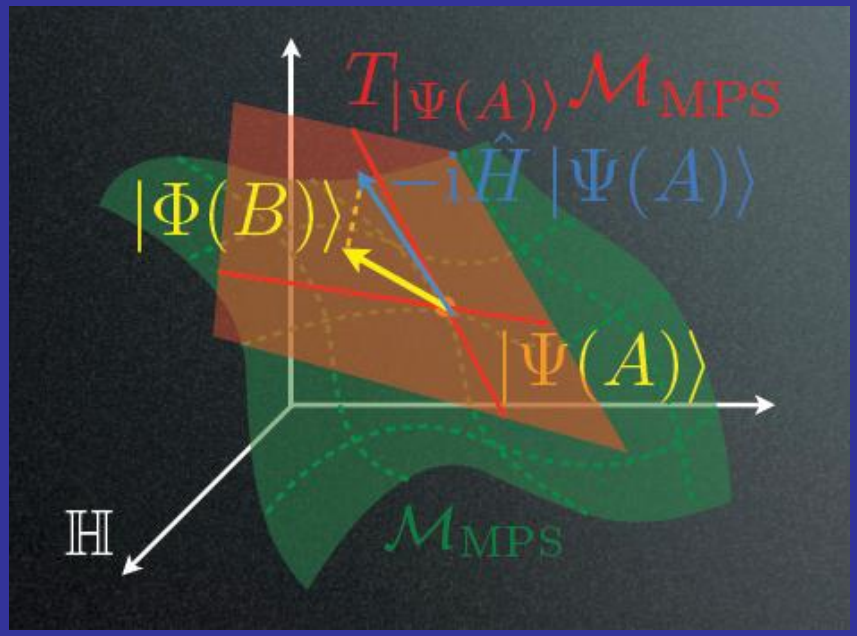
- Gauge degrees of freedom can be chosen such that the Gram matrix of the tangent space is flat (metric is identity).

$$\underbrace{\langle\partial_j\psi|\partial_i\psi\rangle}_{\text{Gram matrix}}\ \dot{A}^i = -i\langle\partial_j\psi|\hat{\mathcal{H}}|\psi\rangle$$

- TDVP approach allows for time evolution with MPS; opposed to other time-dependent DMRG methods, this is
    - Globally optimal
    - Respects all symmetries
    - Yields tangent plane for excitations
    - Allows to find ground states very efficiently

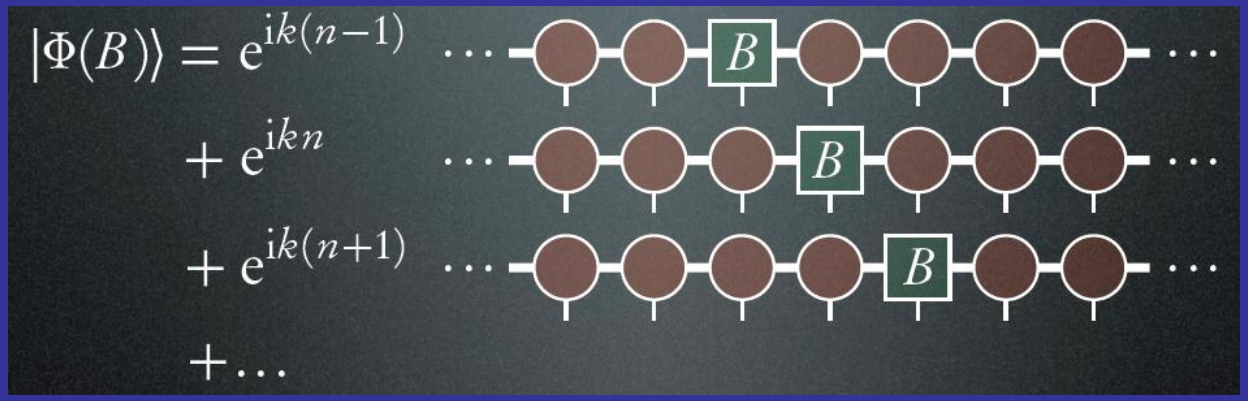
Tangent planes and excitations

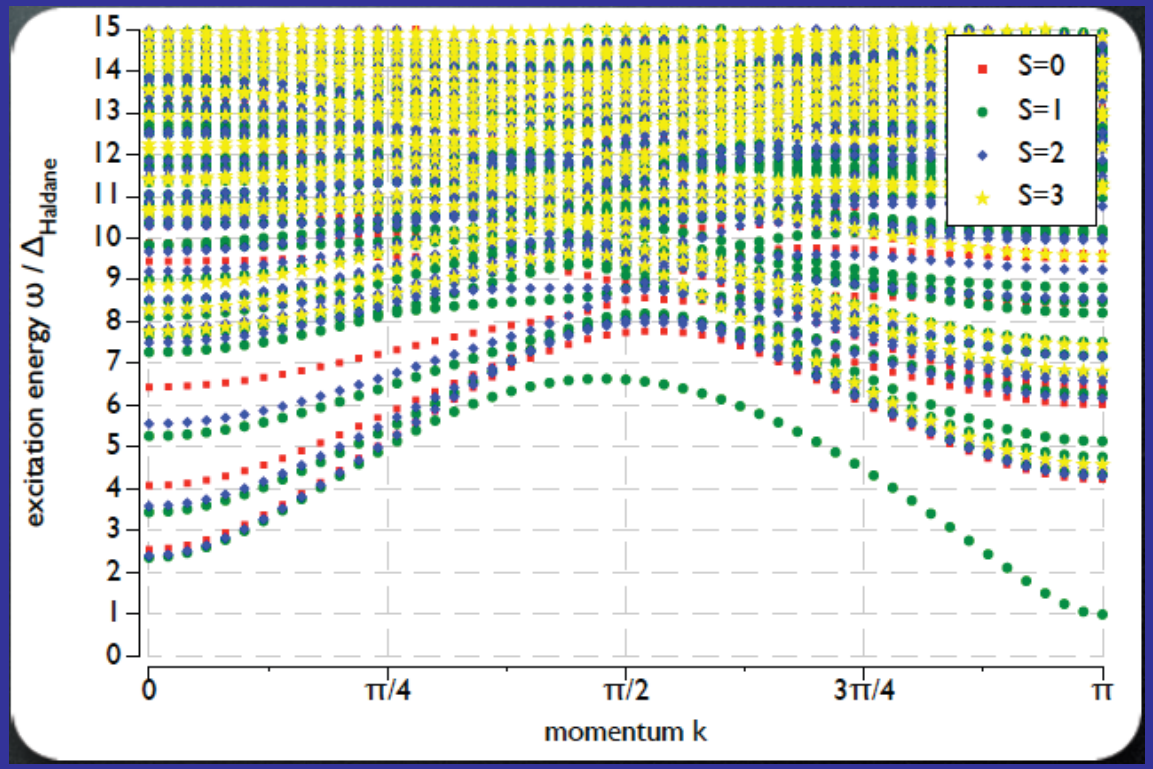
- Stationary points of TDVP correspond to variational minima; the natural thing is now to linearize the physics around those points:
  - The tangent vectors form a linear subspace, so we can project the Hamiltonian on is vector space, and we get an effective quadratic Hamiltonian (linear terms vanish)



Excitations in the tangent plane

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





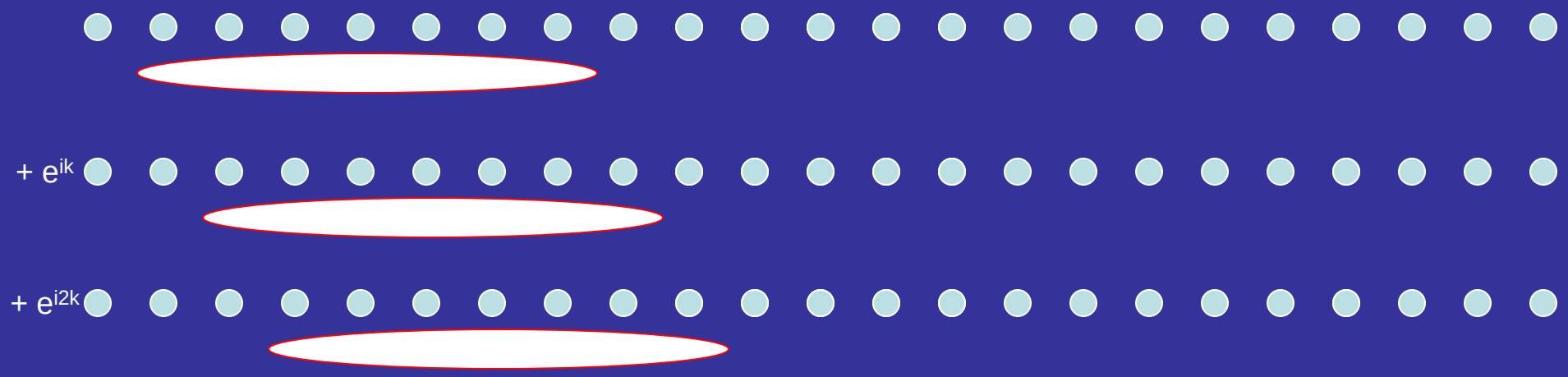
Spin 1 Heisenberg model

$$\Delta^{(\infty)}_{\text{Haldane}} = 0.410479248463^{+6\times10^{-12}}_{-3\times10^{-12}}.$$

Excitations

- Why does this Feynman-Bijl type ansatz for excitations work so well?

- Using methods similar to the ones to prove area laws for gapped 1D systems, it is possible to prove that all isolated elementary excitations can be obtained by acting locally with an operator on the ground state:



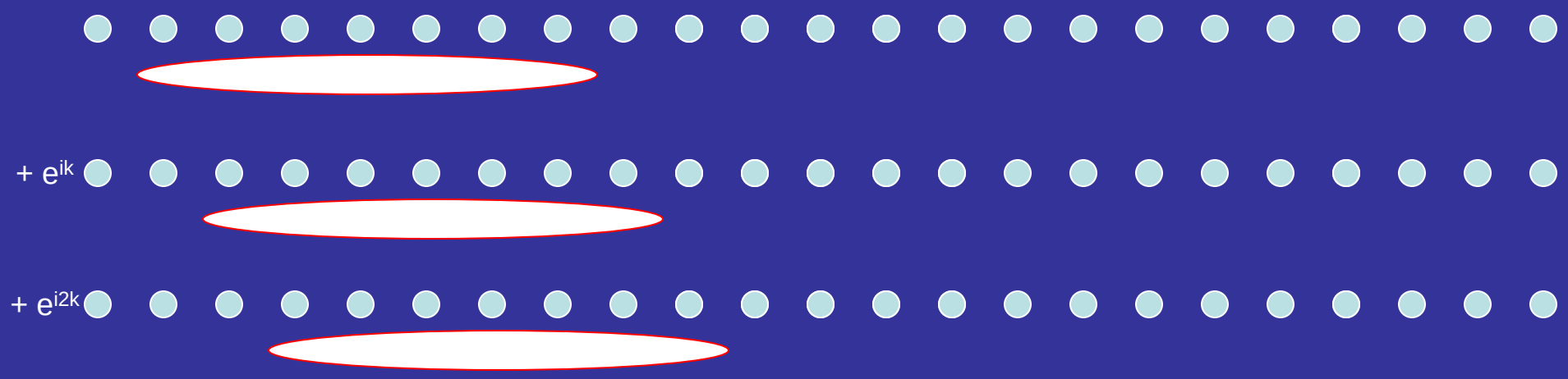
- The length on which those blocks have to act is proportional to the gap between the 1-particle band and the continuum band above it
  - This is a non-relativistic analogue of result of Fredenhagen et al. that elementary particles in QFT are local; instead of light cone, we use Lieb-Robinson bounds

- This is somehow amazing: knowing ground state allows to find all low-lying excited states!

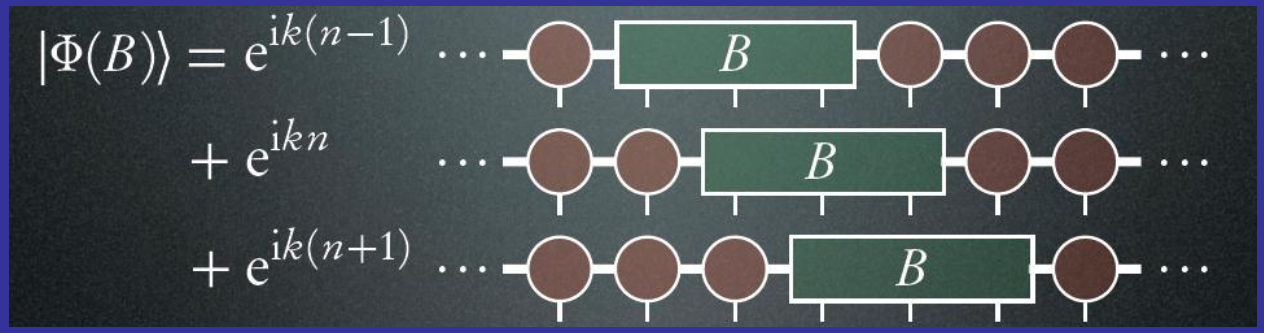
J. Haegeman, S. Michelakis, B. Nachtergaele, T. Osborne, N. Schuch, FV '12

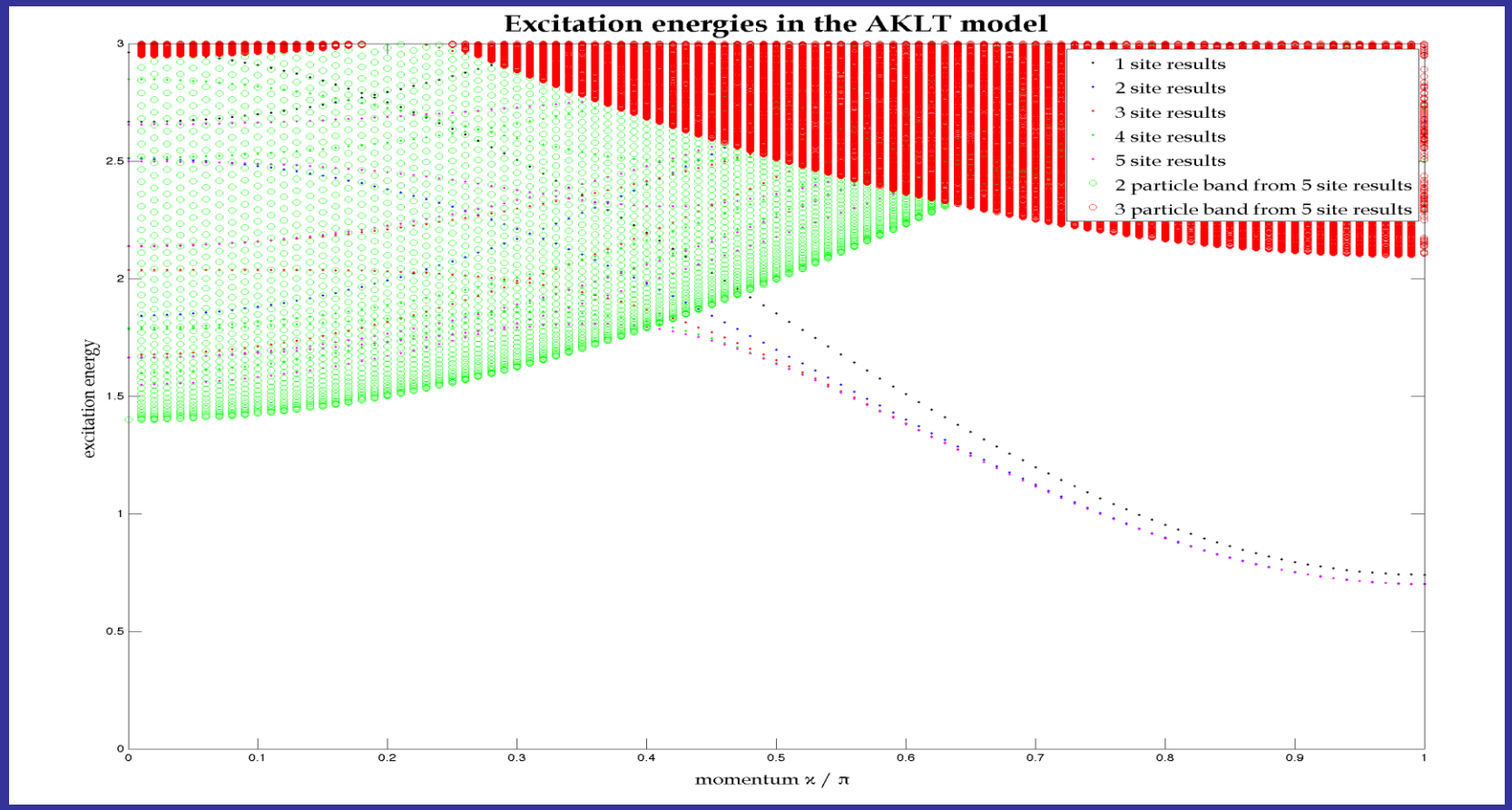
Entanglement entropy of quasi-particle states

- Because of this local construction, the entanglement entropy of the quasi-particle states is exactly given by the entanglement entropy of the ground state + 1 (in log2 units)

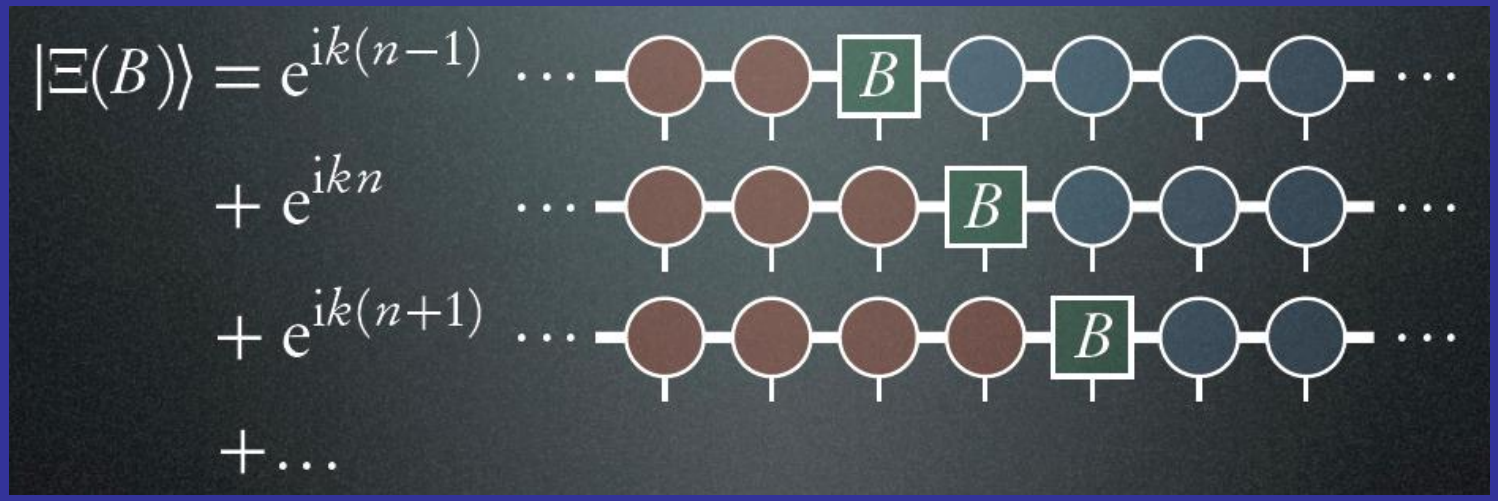


Spin 1 AKLT model





- In the case of symmetry breaking, elementary excitations are typically domain walls between the two phases: topological nontrivial excitations (cfr. Mandelstam ansatz)



Spin 1 XXZ

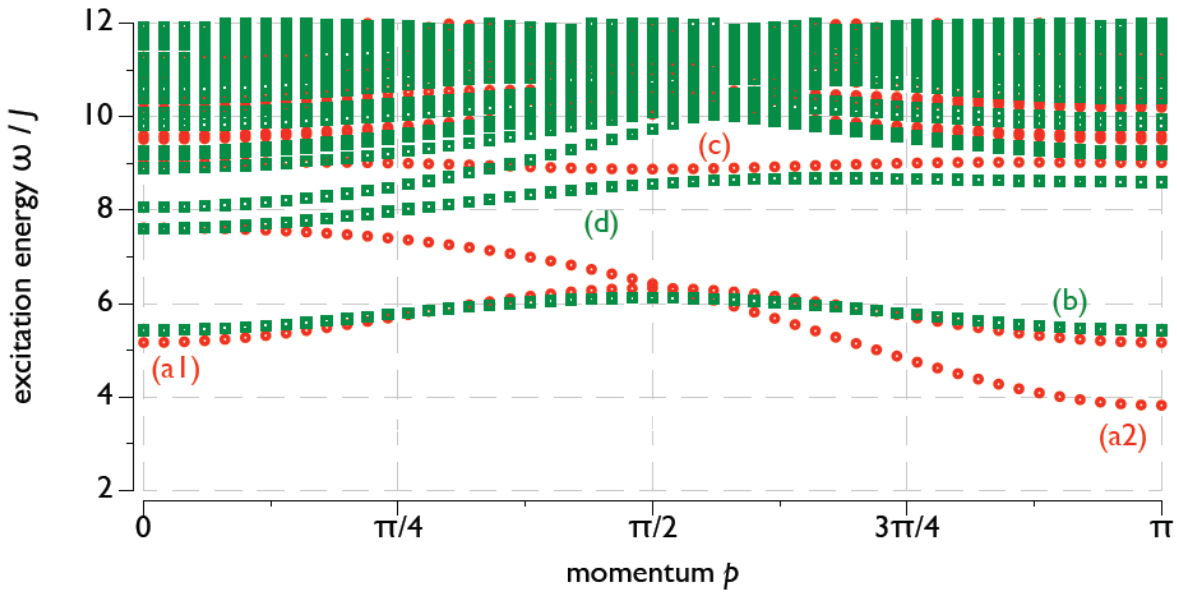


Figure 3.20: Spectrum of the lowest lying excitations of the $S = 1$ XXZ antiferromagnet with anisotropy parameter $\Delta = 3$ at $D = 32$. Red circles indicate topologically non-trivial excitations whereas green squares indicate topologically trivial excitations.

(a) kinks with $\omega = 2\Delta J$: $|\cdots\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\cdots\rangle$ (a1) and $|\cdots\uparrow\downarrow\uparrow 0\downarrow\uparrow\cdots\rangle$ (a2)

(b) spin deviation state with $\omega = 2\Delta J$: $|\cdots\uparrow\downarrow\uparrow 0\uparrow\downarrow\cdots\rangle$

(c) topologically non-trivial bound state with $\omega = 3\Delta J$: $|\cdots\uparrow\downarrow 00\downarrow\uparrow\cdots\rangle$

(d) topologically trivial bound state with $\omega = 3\Delta J$: $|\cdots\uparrow\downarrow 00\uparrow\downarrow\cdots\rangle$

Variational principle for quantum field theories?

- Is it possible to systematically parameterize the low-energy sector of all quantum field theories, just like we did for lattice systems, but without putting it on the lattice?
  - Would open the door to novel non-perturbative approaches for relativistic theories
  - Would allow for a systematic description of the experiments with cold gases (without having to define Hubbard-type band etc.)
  - Why not putting it on a lattice? MPS has finite correlation length!
- One of Feynman's last papers: "Difficulties in Applying the Variational Principle to Quantum Field Theories"
  - "… I didn't get anywhere. So I want to take, for the sake of arguments, a very strong view – which is stronger than I really believe – and argue that it is no damn good at all! "

Feynman Objection I: Sensitivity to High Frequencies

- Energy contributions to the total energy of the high frequency modes are much more important than the low-energy ones

- Therefore any variational method will try to get the high-frequencies right, even at the cost of getting low-energy behaviour wrong
  - "… what happens when I allow it to adjust its parameter (to lower the total energy), is it improves the imperfect function I was using at the high frequencies…"

- This is obviously not what we want!
  - We are interested in long-range low-energy physics, this is the point of a quantum field theory

Feynman Objection II: Only exponential trial states

- For atoms, very good variational wavefunctions are of the form

$$\psi(x) \approx \left(1-\beta x^4\right)\exp\left(-\alpha x^2\right)$$

- This is not possible in the case of QFT, as the dimensions do not fit in formulae like

$$\psi(\varphi) \approx \left(1-\beta\int \phi(x)^4 dx\right)\exp\left(-\int\int \phi(x)K(x,y)\varphi(y)dxdy\right)$$

the wavefunction has to be “size extensive”

- What we want instead is corrections of the form $\exp\left(-\beta\int \phi(x)^4 dx\right)$ but then we have to evaluate non-Gaussian functional integrals which is extremely hard to do with good enough precision

Feynman's visionary suggestion as a way out:

"Now, in field theory, what's going on over here and what's going on over there and all over space is more or less the same. Why do we have to keep track in our functional of all things going on over there while we are looking at the things that are going on over here? ... It's really quite insane, actually: we are trying to find the energy by taking the expectation value of an operator which is located here and we present ourselves with a functional which is dependent on everything all over the map. That's something wrong. Maybe there is some way to surround the object, or the region where we want to calculate things, by a surface and describe what things are coming in across the surface. It tells us everything that's going on outside."

"I think it should be possible some day to describe field theory in some other way than with the wave functions and amplitudes. It might be something like the density matrices where you concentrate on quantities in a given locality and in order to start to talk about it you don't immediately have to talk about what's going on everywhere else ..."

This is actually exactly what S. White did with the "density matrix renormalization group" DMRG, which is now understood as a variational method within the class of MPS

MPS in the continuum limit:

$$|\chi\rangle = \mathrm{Tr}_{aux}\left[\mathcal{P}e^{\int_0^L dx\left[Q(x)\otimes\mathbb{1}+R(x)\otimes\hat{\psi}^\dagger(x)\right]}\right]|\Omega\rangle$$

$$[\hat{\psi}(x),\hat{\psi}(y)^\dagger] = \delta(x-y)$$

Q(x), R(x) are DxD matrices acting on an auxiliary Hilbert space. The wavefunction is automatically normalized and the total number of parameters is exactly D^2 if we use the gauge condition

$$Q = -\frac{1}{2}R^\dagger R - iH$$

FV, Cirac, PRL 2010

cMPS in second quantization

$$|\chi\rangle = \sum_{n=0}^{\infty} \int_{0<x_1<\ldots<x_n<L} dx_1 \ldots dx_n \phi_n \hat{\psi}^\dagger(x_1) \ldots \hat{\psi}^\dagger(x_n)|\Omega\rangle$$

$$\phi_n = \mathrm{Tr}_{aux}\left[u_Q(x_1,0) R u_Q(x_2,x_1) R \ldots R u_Q(L,x_n)\right]$$

$$u_Q(y,x) = \mathcal{P}\exp\left[\int_x^y Q(x)dx\right]$$

$$Q = -\frac{1}{2}R^\dagger R - iH$$

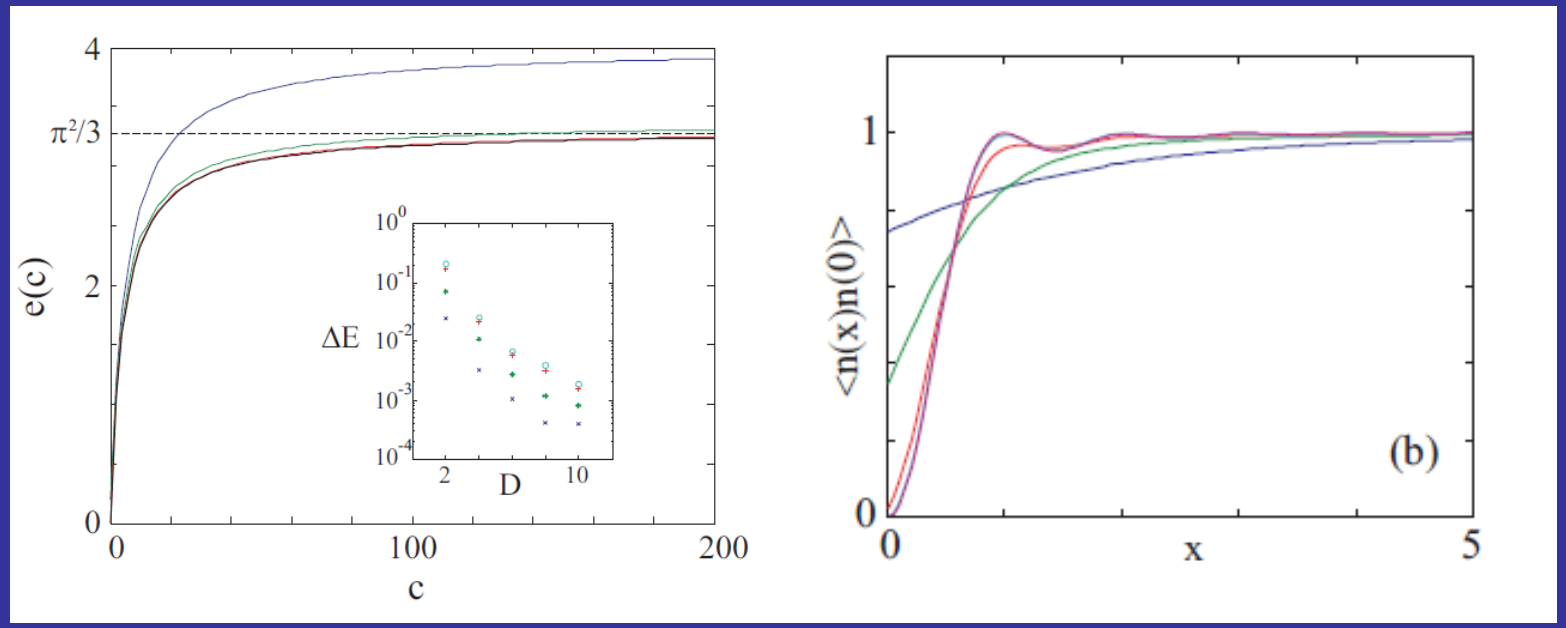
- Where is the density matrix?
  - Lindblad evolution instead of CP-map:

$$\frac{d}{dx}\rho(x) = -i[\tilde{H},\rho(x)] + R\rho(x)R^\dagger - \frac{1}{2}\left[R^\dagger R, \rho(x)\right]_+$$

  - The density martrix lives on the virtual space, and its eigenvalues are the Schmidt coefficients of the halve-chain: entanglement spectrum!

Example: the Lieb-Liniger model

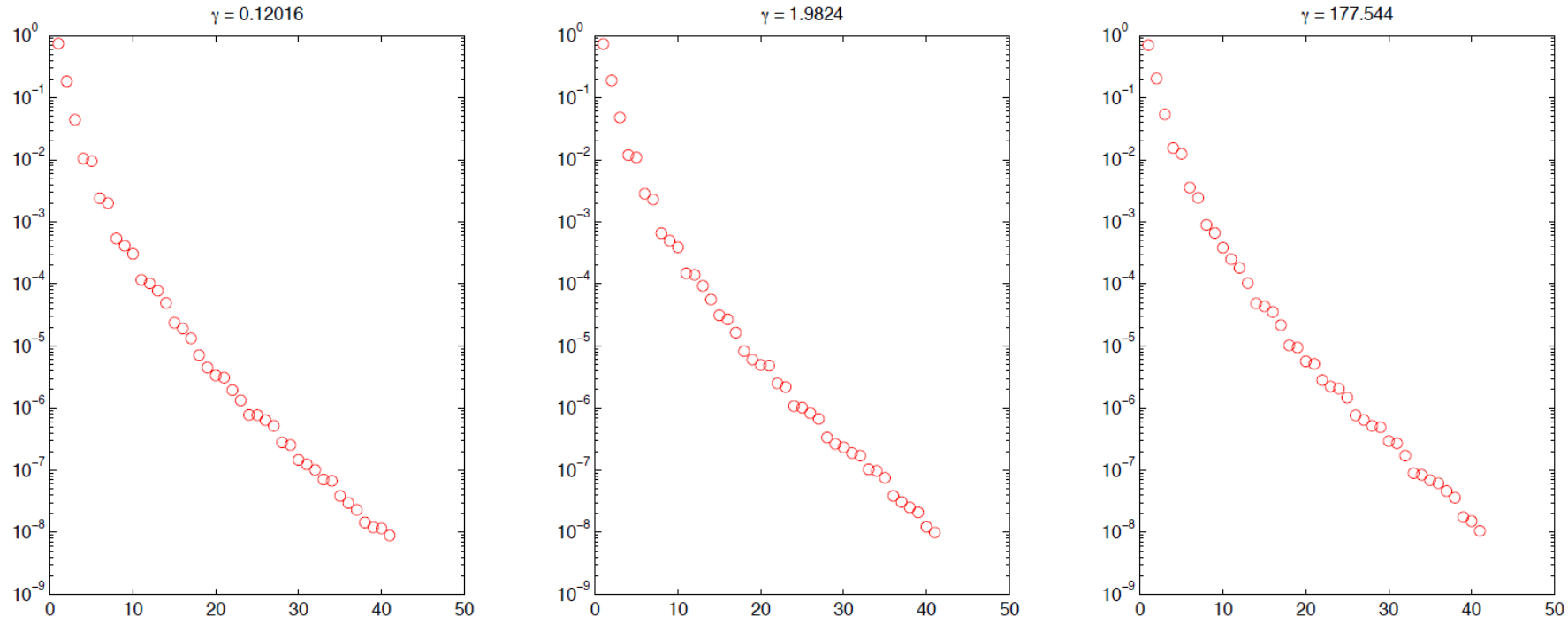
$$\mathcal{H} = \int_{-\infty}^{+\infty} dx \left[\frac{d\hat{\psi}^\dagger(x)}{dx} \frac{d\hat{\psi}(x)}{dx} + c\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x) \right]$$



- Working towards simulating non-translational invariant systems such as interacting bosons / fermions in an external potential (e.g. optical lattices)

Schmidt coefficients / entanglement spectrum for the Lieb-Liniger model:

$$\mathcal{H} = \int_{-\infty}^{+\infty} dx \left[\frac{d\hat{\psi}^\dagger(x)}{dx} \frac{d\hat{\psi}(x)}{dx} + c\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x) \right]$$



Overcoming objection 1 of Feynman: high frequencies in cMPS

- Expectation value of the non-relativistic kinetic energy:

$$\langle \hat{\psi}(x)^\dagger \left[-\frac{d^2}{dx^2} \right] \hat{\psi}(x) \rangle \;=\; \mathrm{Tr}\left[e^{TL}([Q,R] \otimes [\bar{Q},\bar{R}]) \right]$$

  - This is automatically bounded if all matrices involved are bounded in norm

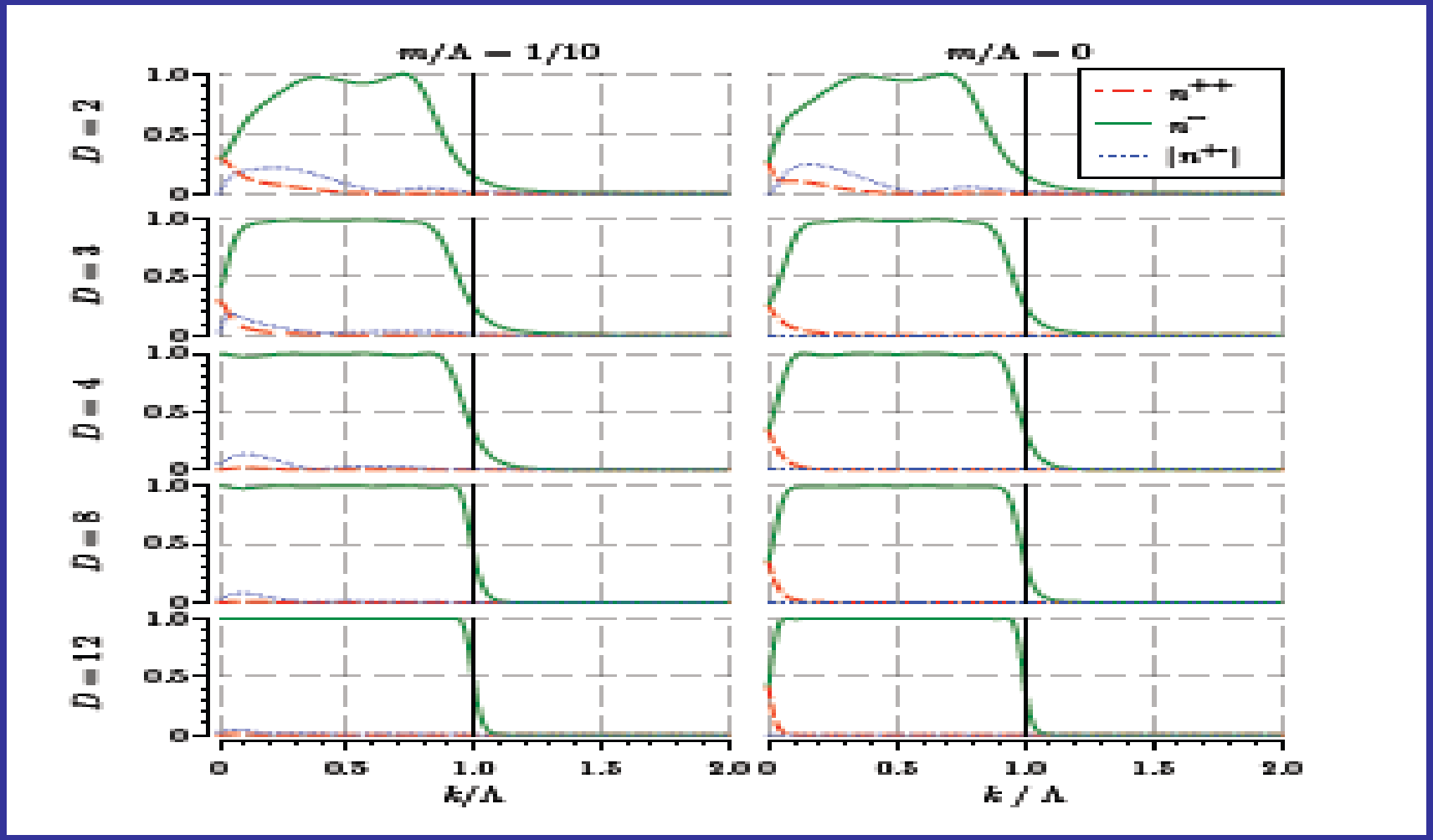
  - If a cMPS wavefunction is such that its second order derivative is continuous, then the expectation value of its high-frequency components scales like

$$n(k) \approx \frac{1}{k^4}$$

    - This imposes an effective high-energy cut-off as all expectation values become finite; hence we can go and look at relativistic theories!

Haegeman, Cirac, Osborne, Verschelde, FV PRL '10

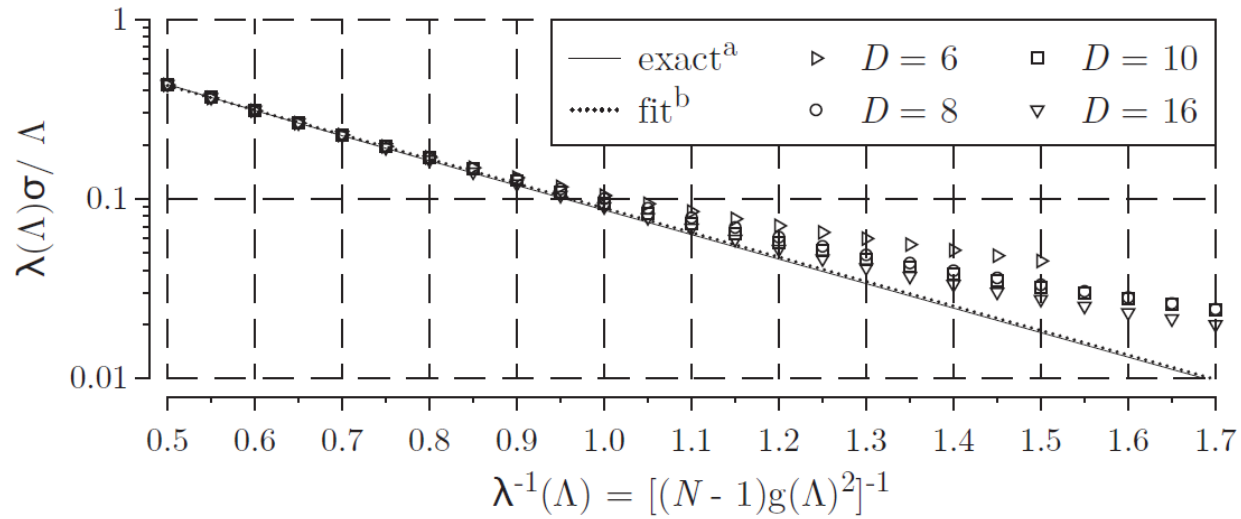
Example: free Dirac fermions with cMPS



Simulation of free Dirac fermions by introducing an effective cut-off; plotted is n(k) obtained as the Fourier transform of the 1-particle density matrix $\langle\chi|\hat{\psi}^\dagger_\alpha(x)\hat{\psi}_\beta(x')|\chi\rangle = C_{\alpha,\beta}(x-x')$

Gross Neveu model using cMPS

$$\hat{h}_{GN} = -\frac{\mathrm{i}}{2}\hat{\psi}_a^\dagger \sigma^y \frac{\mathrm{d}\hat{\psi}_a}{\mathrm{d}x} + \frac{\mathrm{i}}{2}\frac{\mathrm{d}\hat{\psi}_a^\dagger}{\mathrm{d}x}(x)\sigma^y \hat{\psi}_a(x) - \frac{g^2}{2} : (\hat{\psi}_a^\dagger \sigma^z \hat{\psi}_a)^2 :$$



Expectation value of $\sigma = \langle\chi|\,\hat{\psi}^\dagger\sigma^z\hat{\psi}\,|\chi\rangle$ in the Gross-Neveu model as function of $\lambda(\Lambda)$ for $N = \infty$.

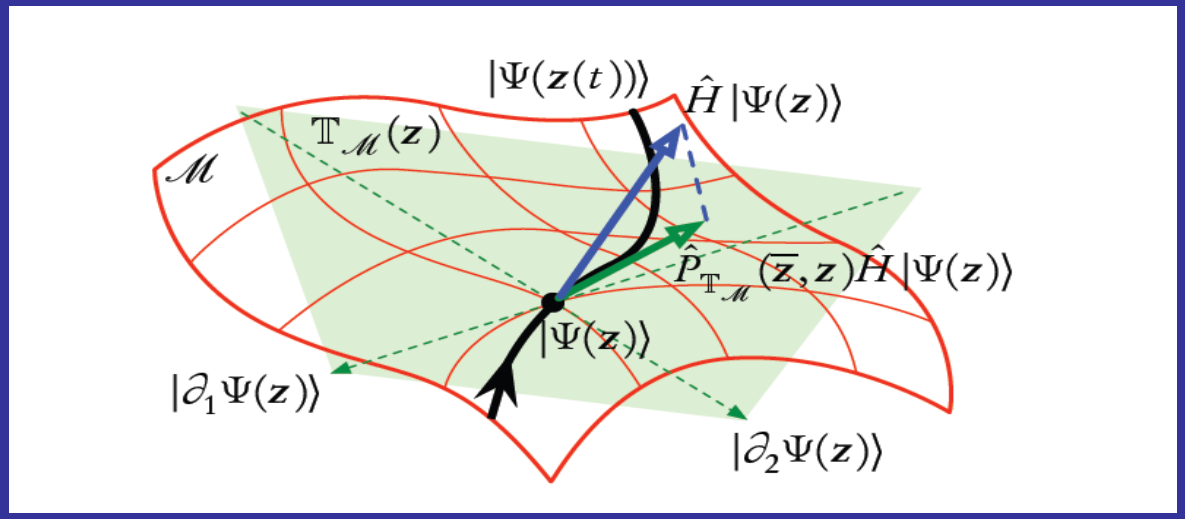
[a] Exact result $|\lambda\sigma|/\Lambda \approx 2\mathrm{e}^{-\pi/\lambda}$ follows from Eq. (3)

[b] A fit of the form $c_1 e^{-c_2/\lambda}$ to th[illegible] or $\lambda^{-1} \leq 1$ at $D = 16$ results in $c_2 = 3.142^{+0.047}_{-0.047}$ and $c_1 = 2.057^{+0.074}_{-0.072}$.

Haegeman, Cirac, Osborne, Verschelde, FV PRL '10

The time-dependent variational principle for cmps

- The question: how to optimize those matrices / tensors?
- cMPS form a low-dimensional manifold in the huge Hilbert space
  - It has a very interesting geometrical structure
  - To find ground states, we can evolve in imaginary time: guaranteed to converge to the ground state
  - Time-dependent variational principle:



$$y = argmin_y \left\| \mathcal{H}\psi - \sum_i y_i \frac{\partial \psi}{\partial z_i} \right\| \qquad \Rightarrow \qquad \frac{\partial z_i}{\partial t} = -y_i = f(z)$$

- The linear differential equation (Schrodinger equation) in an exponentially large Hilbert space is mapped to a nonlinear differential equation in a small dimensional manifold!

Case of D=1: Gross Pitaevskii / nonlinear Schrodinger equation

$$|\chi\rangle = \mathrm{Tr}_{aux}\left[\mathcal{P}e^{\int_0^L dx\left[Q(x)\otimes\mathbb{1}+R(x)\otimes\hat{\psi}^\dagger(x)\right]}\right]|\Omega\rangle$$

$$H = \sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\mathbf{r}_i^2}+V(\mathbf{r}_i)\right)+\sum_{i<j}\frac{4\pi\hbar^2 a_s}{m}\delta(\mathbf{r}_i-\mathbf{r}_j),$$

$$\Rightarrow\ ih\frac{\partial R}{\partial t} = (-\Delta + V(x) + g|R|^2)R$$

Quantum Gross-Pitaevskii equations

- cMPS formalism yields the natural generalization of the GP:

$$\frac{\partial}{\partial x}E_L(x) = R(x)^\dagger E_L(x)R(x) + \left(\dot{R}(x)^\dagger \rho_L(x)\dot{R}(x) + c(R^2(x))\dagger \rho_L(x)R^2(x)\right)$$
$$\frac{\partial}{\partial x}E_R(x) = R(x)E_R(x)R(x)^\dagger + \left(\dot{R}(x)\rho_R(x)\dot{R}(x)^\dagger + cR^2(x)\rho_L(x)(R^2(x))^\dagger\right)$$

$$\frac{d}{dt}\left(\rho_L(x)R(x)\rho_R(x)\right) = E_L(x)R(x)\rho_R(x) + \rho_L(x)R(x)E_R(x) + \left(-\rho_L(x)R''(x)\rho_R(x) + c\rho_L(x)R^2(x)\rho_R(x)R(x)^\dagger + cR(x)\rho_L(x)R^2(x)\rho_R(x)\right)$$

  - Matrix (“quantum”) version of Gross-Pitaevskii equation!
  - use of gauge degrees of freedom allows to make those equations strictly local and hence easy to integrate using standard techniques

Elementary excitations

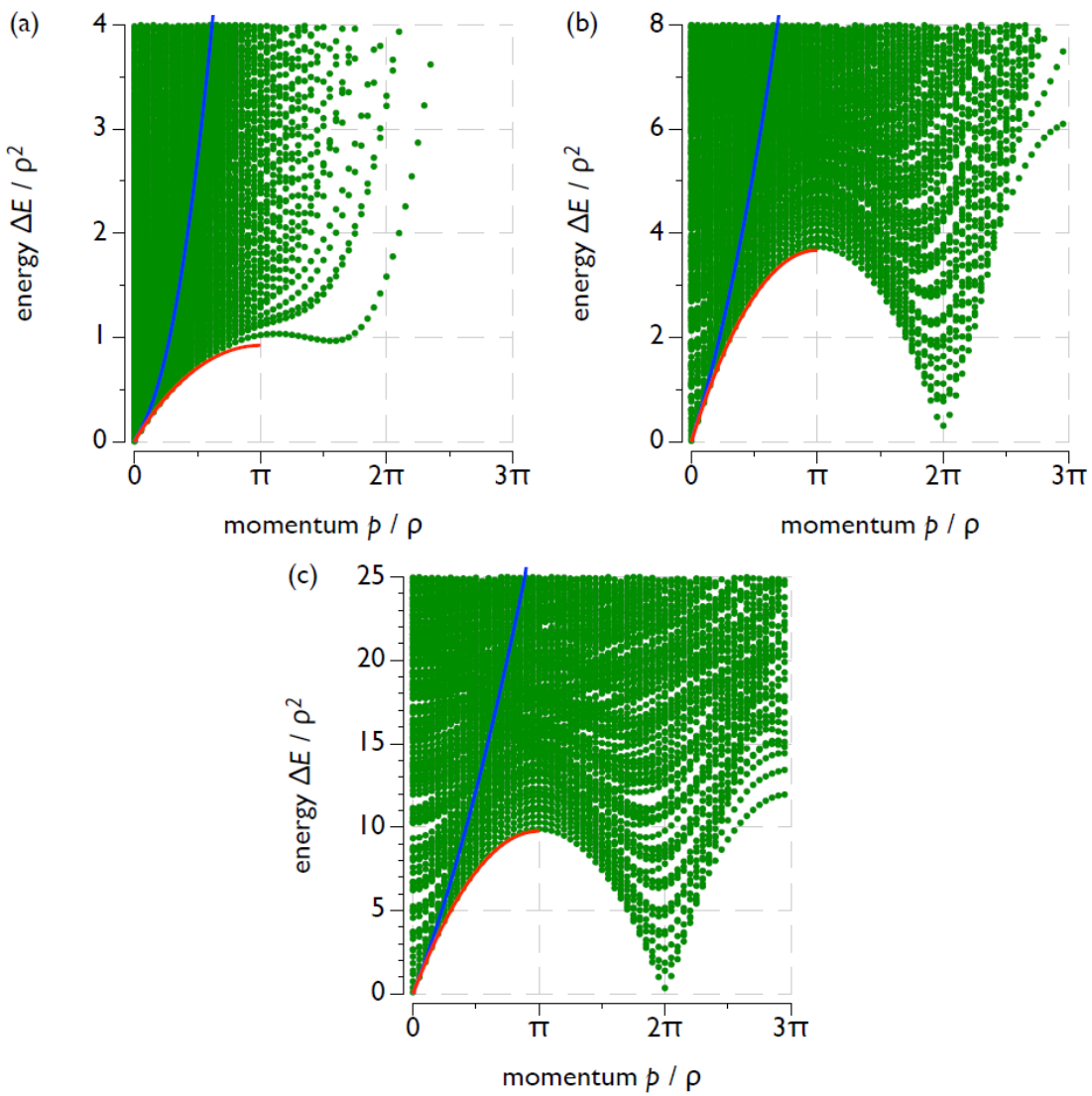
- Ground state physics is only the start: this is the vacuum!
  - Real fun starts when we can look at elementary excitations (quasi-particles).

- Note that is well understood how to get excitations on top of Gross-Pitaevskii: construct an effective quadratic theory (Bogoliubov-deGennes)

$$|\Xi_p(V,W)\rangle = \int_{-\infty}^{+\infty} \mathrm{d}x\, \mathrm{e}^{\mathrm{i}px} \boldsymbol{v}_{\mathrm{L}}^{\dagger} \hat{U}_1(-\infty,x) \left(V \otimes \hat{\mathbb{1}} + W \otimes \hat{\psi}^{\dagger}(x) \right) \hat{U}_2(x,+\infty) \boldsymbol{v}_{\mathrm{R}} |\Omega\rangle ,$$

$$\hat{U}_1(y,z) = \mathcal{P}\exp\left[\int_y^z \mathrm{d}x\, Q_1 \otimes \hat{\mathbb{1}} + R_1 \otimes \hat{\psi}^{\dagger}(x)\right], \qquad \hat{U}_2(y,z) = \mathcal{P}\exp\left[\int_y^z \mathrm{d}x\, Q_2 \otimes \hat{\mathbb{1}} + R_2 \otimes \hat{\psi}^{\dagger}(x)\right]$$

  - As this wavefunction is linear in V,W, we obtain an effective quadratic theory in the matrices V,W , and this yields D^2 eigenstates

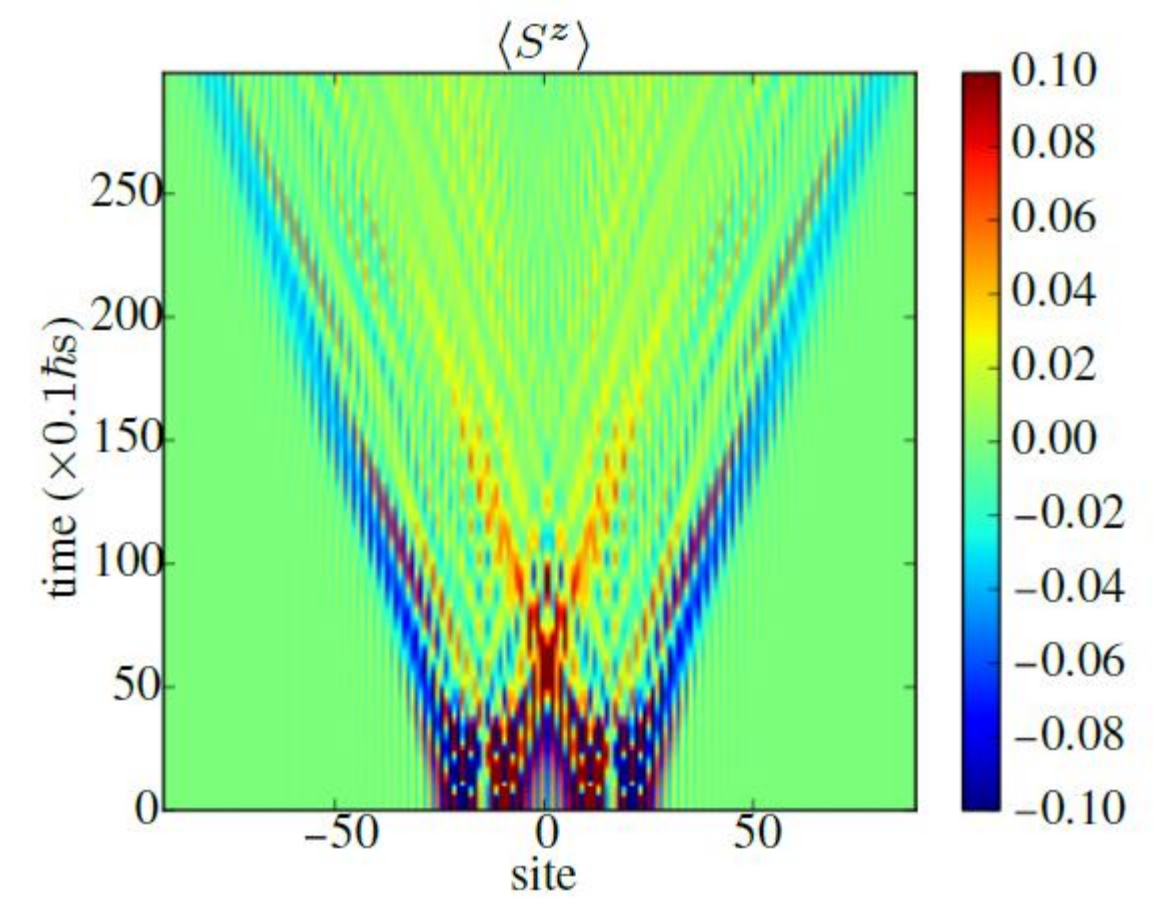


igure 4.5: Spectra obtained with our ansatz $|\Phi(V, W)\rangle$ with bond dimension $D = 33$, for $\gamma \approx 0.12$ (a), $\gamma \approx 1.98$ (b) and ≈ 337.47 (c). Also shown are the 'elementary excitations' of type I (blue line) and type II (red line) according to [16].

Outlook

- Boundary theories for generic quantum spin systems
- Classification of topological phases of matter by symmetries of tensors (Wen et al.)
- Simulating Hubbard type models
- Continuous PEPS: quantum field theory with wavefunctions
- Scattering of quasi-particles : seeing this in real time
- Generic constructions of effective theories
- Lieb-Robinson bounds for continuum theories
- …

Real-time evolution: scattering experiments



Milsted et al., 2012

Conclusions

- The variational principle makes sense for many-body quantum systems: physical (low-energy) states live in a tiny corner of Hilbert space

- In case of gapped 1 dimensional quantum systems, this corner seems to have been identified
  - Classification of phases, symmetry protected order, …

- Holographic principle: relevant degrees of freedom live in a theory of one dimension lower

- It is possible to develop quantum field theory with wavefunctions in real-space
  - Continuous Matrix Product States seem to capture the low-energy physics of 1+1 dimensional quantum field theories (both relativistic and non-relativistic)

- Intriguing connections between quantum field theory, quantum measurement theory, dissipative non-equilibrium phenomena and the holographic principle