Projected Entangled-Pair States: properties and applications

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Pisa, 14 December 2004

Many-body quantum systems

- Many-body quantum systems are difficult to describe.

$$|\Psi\rangle$$

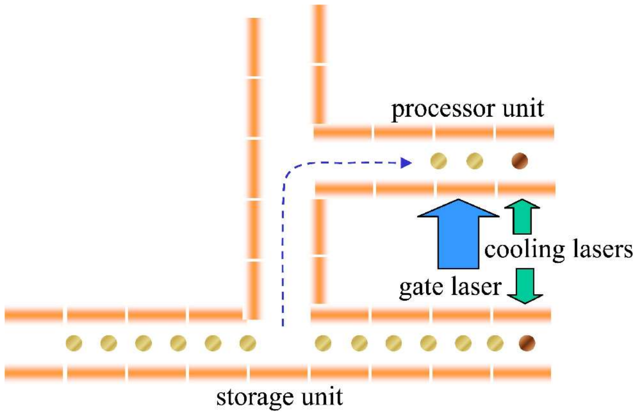
$$|\Psi\rangle = \sum c_{i_1 \ldots i_N} |i_1, \ldots, i_N\rangle$$

We need 2^N coefficients to represent a state.

- To determine physical quantitites (expectation values) an exponential number of computations is required.

Solutions:

- One may use a quantum computer (Lloyd):

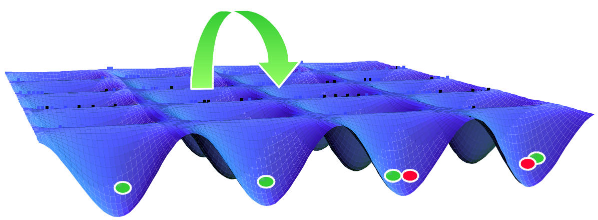


$$U = e^{-iHt} \approx e^{-iH_1 t_1} e^{-iH_2 t_2} \ldots e^{-iH_N t_N}$$

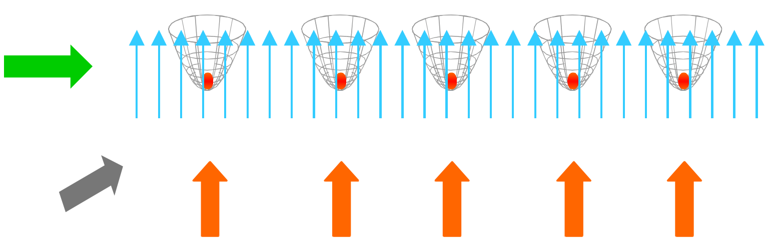
For example, with trapped ions (NIST, Innsbruck)

Quantum simulation may be the first application of a quantum computer.

- One may use an analogue system (Feynman):



(e.g. Hoffstäter, Cirac, Zoller, Demler, and Lukin)



(Porras and Cirac)

- One may try with a classical computer:

Numerical Methods:

- Monte-Carlo methods:

  - It works very well in 1,2, and 3D.

  - It has the „sign" problem:

    Problems with Fermions or frustration cannot be simulated.

  - It is difficult to simulate dynamics.

- Density Matrix Renormalization Group (DMRG): (White 1991).

  - It has no „sign" problem.

  - Works for 1D systems:

    - Ground state in problems with open boundary conditions.
    - Time-dependence for Hamiltonian systems and pure states with OBC.

      (Vidal, White, Scholwöck et al)

    - Finite temperature for infinite homogeneous systems.

      (Nishino)

This talk:

- Motivated by QIT ideas:

  Projected-pair entangled states

- Application: Numerical algorithms:

  QIT ➡ CMP

  1D:

  - Ground state (open boundary conditions) = DMRG.
  - Ground state (periodic boundary conditions).
  - Finite temperature (finite and inhomogeneous).
  - Optimal time-dependent methods.
  - Dissipative systems.
  - Random systems.
  - Excitations and spectral functions.
  - Kondo problems
  - …

  2D and higher dimensions:

- Application: 1-way quantum computing and error correction.
- Physical systems: the chicken and the egg…

Collaborations: D. Porras, J.J. Garcia-Ripoll, V. Murg, B. Paredes (MPQ) Numerics
U. Schollwöck (Aachen), J. von Delft (LMU) Kondo
M.A. Martin-Delgado (Madrid) General
C. Schön, E. Solano and M. Wolf (MPQ) Physical Systems
J.I. Latorre, E. Rico (Barcelona) RG

Many-body quantum systems

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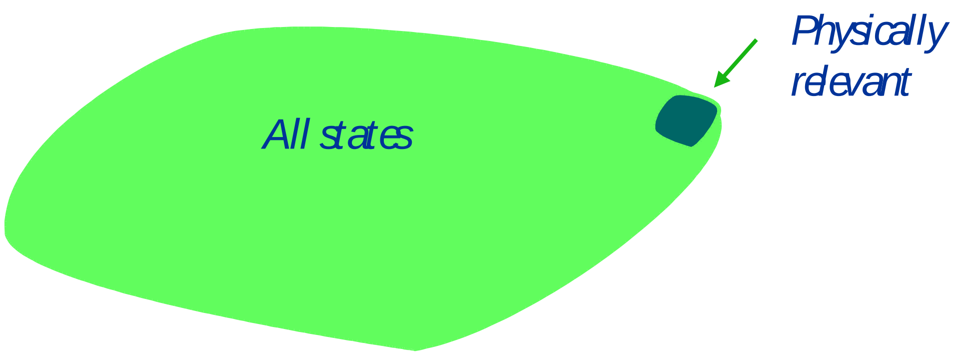
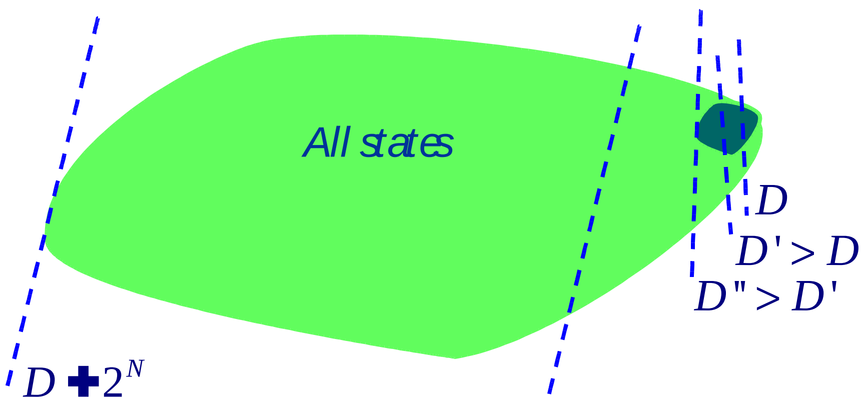


Projected entangled-pair states

- Family of states.
- Important quantity: D: Number of parameters characterizing the state.



- With relatively small D, one can represent physically relevant states.
- One can determine physical properties in an efficient way.

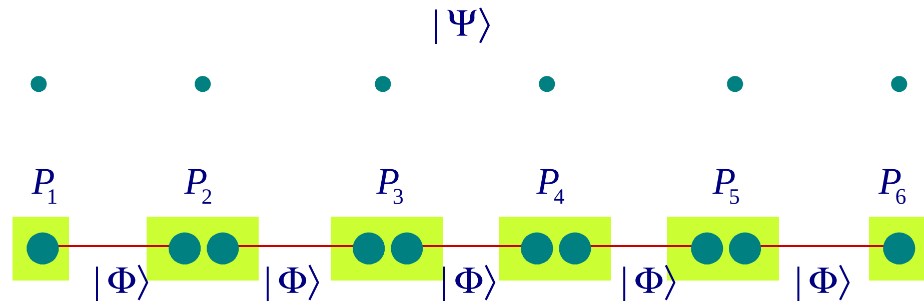
1. Definition

GHZ states:

$$|\mathrm{GHZ}\rangle = |0,0,0\rangle + |1,1,1\rangle$$

where $P = |0\rangle\langle 0,0| + |1\rangle\langle 1,1|$ *maps* $❣^2 \otimes ❣^2 \to ❣^2$

1D states:



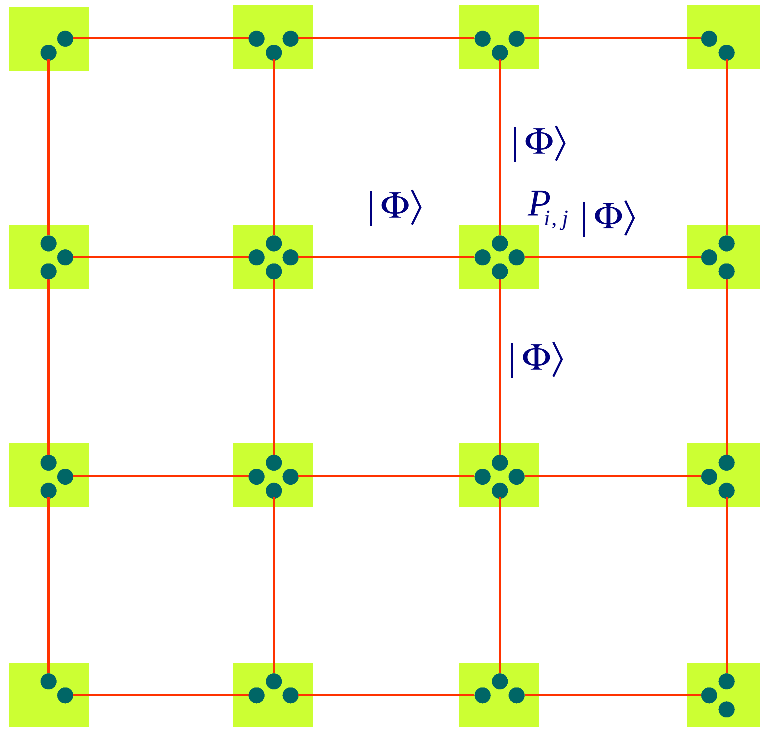
where

● *D-dimensional*

$$|\Phi\rangle = \sum_{m=1}^{D} |m,m\rangle$$ *are maximally entangled states*

$$P_k = \sum_{n=1}^{2} |n\rangle\langle\varphi_n^k|$$ *maps* $❣^D \otimes ❣^D \to ❣^2$

2D states:

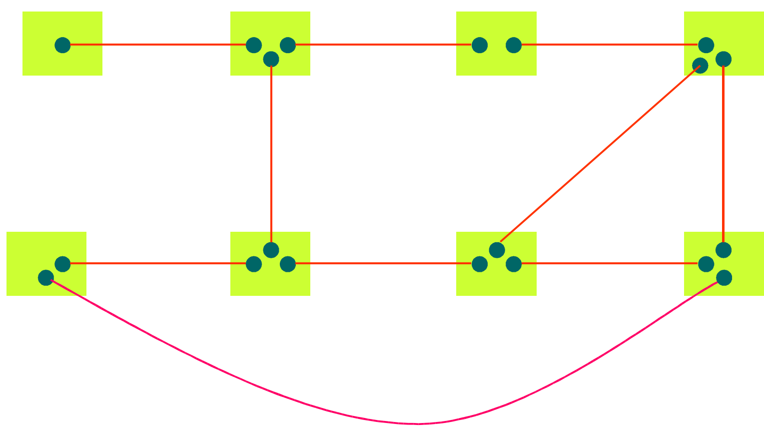


$$P_k = \sum_{n=1}^{2} |n\rangle\langle\varphi_n^k|$$

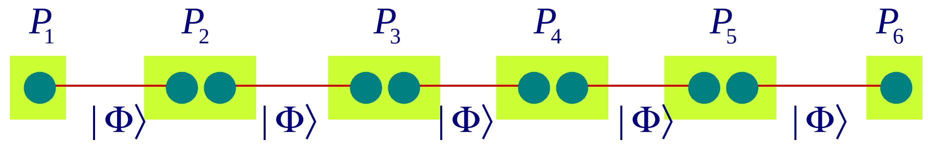
maps

$$\mathbb{C}^D \otimes \mathbb{C}^D \otimes \mathbb{C}^D \otimes \mathbb{C}^D \to \mathbb{C}^2$$

General:



Mixed PEPS



where the P are now Completely Positive Maps

$$P_k : B\left[\mathbb{C}^D \otimes \mathbb{C}^D\right] \rightarrow B\left[\mathbb{C}^2\right]$$

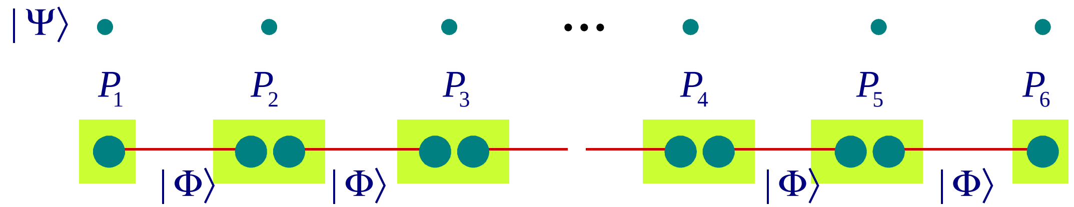
We can also use purifications

$|\Psi_{\mathrm{PEPS}}\rangle$

$$\rho = \mathrm{Tr}\left(|\Psi_{\mathrm{PEPS}}\rangle\langle\Psi_{\mathrm{PEPS}}|\right)$$

2. Properties:

- They are complete:



Proof: via teleportation

- They are ground state of local Hamiltonians: $H|\Psi\rangle = E_0|\Psi\rangle$

- They satisfy the area theorem: a requirement for describing physical states.

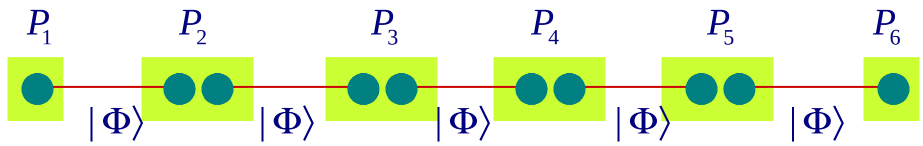
- In 1D they coincide with: Finitely correlated states (Fannes et al)
Matrix product states (Römer and Ostlund)

$$P_k = \sum_{n=1}^{2} |n\rangle\langle\varphi_n^k| = \sum_{i_k=1}^{2} \left[A_k^{i_k}\right]_{\alpha,\beta} |i_k\rangle\langle\alpha,\beta| \Rightarrow |\Psi\rangle = \sum_{i_1,\dots,i_N=0}^{1} \mathrm{Tr}\left(A_1^{i_1}A_2^{i_2}\dots A_N^{i_N}\right)|i_1,\dots,i_N\rangle$$

- In 2D they extend FCS and MPS.

- Expectation values of observables have a simple form:

PEPS in 1D



$$P_k = \sum_{n=1}^{2} |n\rangle\langle\varphi_n^k| = \sum_{i_k=1}^{2} \left[A_k^{i_k}\right]_{\alpha,\beta} |i_k\rangle\langle\alpha,\beta| \quad \Rightarrow \quad |\Psi\rangle = \sum_{i_1,\dots,i_N=0}^{1} \mathrm{Tr}\left(A_1^{i_1} A_2^{i_2} \dots A_N^{i_N}\right) |i_1,\dots,i_N\rangle$$

Finitely correlated states (Fannes et al)
Matrix product states (Römer and Ostlund)

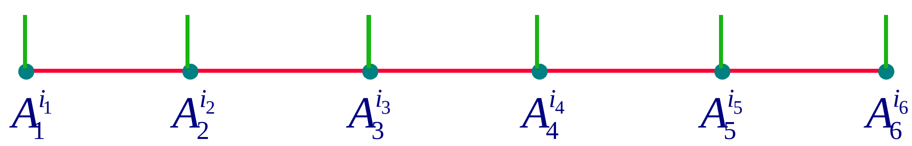
$D^2 \times D^2$ *matrices*

- *Correlation functions:*

$$\langle\sigma_x^i \sigma_y^j\rangle = \frac{\mathrm{Tr}\left[E_1 E_2 \dots X_i E_{i+1} \dots Y_j E_{j+1} \dots E_N\right]}{\mathrm{Tr}\left[E_1 E_2 \dots E_N\right]}$$

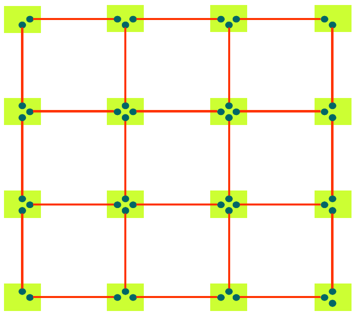
Representation

- *States:*



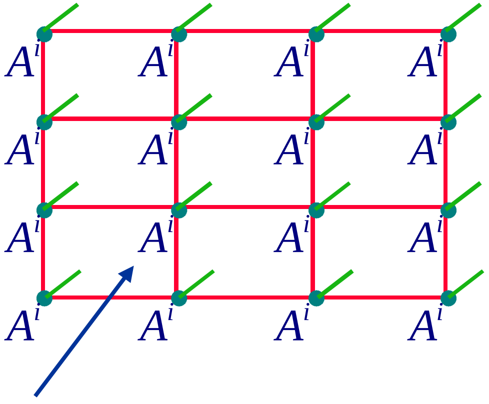
- *Correlation functions:*

PEPS in 2D



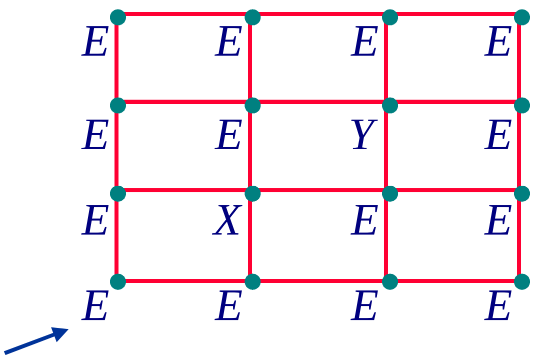
Representation

States:



$D\times D\times D\times D\times 2$ tensor

Correlation functions:



$D^2\times D^2\times D^2\times D^2$ tensor

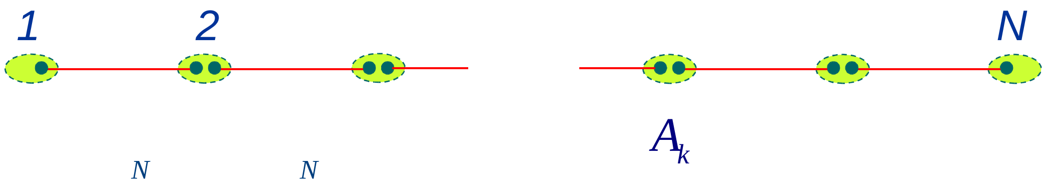
Problem: when contracting, the indices proliferate.

This happens for tensor with more than 2 indices.

$$\sum_{\alpha} E_{\alpha\beta\gamma\delta} E_{\alpha\varepsilon\kappa\lambda} = M_{\beta\gamma\delta\varepsilon\kappa\lambda}$$

3. Ground state (1D)

IDEA: For a given D, find the optimal A *which minimizes the energy.*



Hamiltonian: $$H = \sum_{x=1}^{N} H_x + \sum_{x,y=1}^{N} H_{x,y} + \ldots$$

We want to find $$\min_{\Psi \text{ PEPS}} \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_0$$

Procedure:

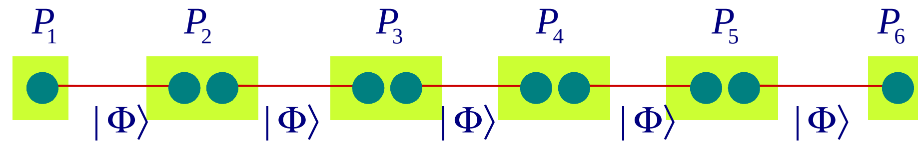
- *Fix all A's except for one:* A_k
- *Minimize with respect to* A_k

One has to solve a (generalized) eigenvalue problem

- *Iterate:*

- *The process converges.*

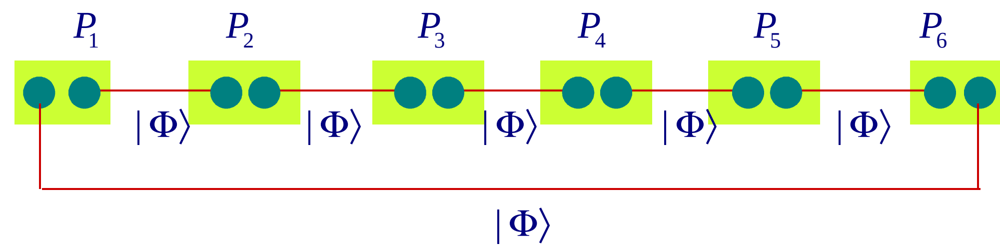
1) Open boundary conditions:



It coincides with DMRG

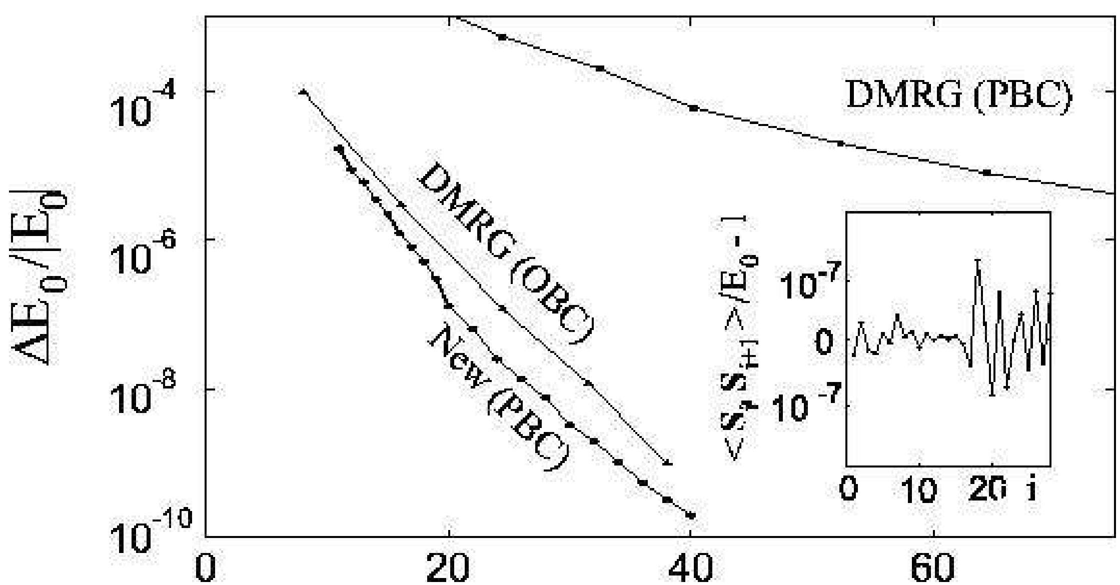
2) Periodic boundary conditions:

(Verstraete, Porras, Cirac, PRL 2004)



It outperforms DMRG

$$H=\sum_{\langle k,j\rangle}\left(\sigma_x^k\sigma_x^j+\sigma_y^k\sigma_y^j+\sigma_z^k\sigma_z^j\right)$$



Translationally invariant systems: Excitations

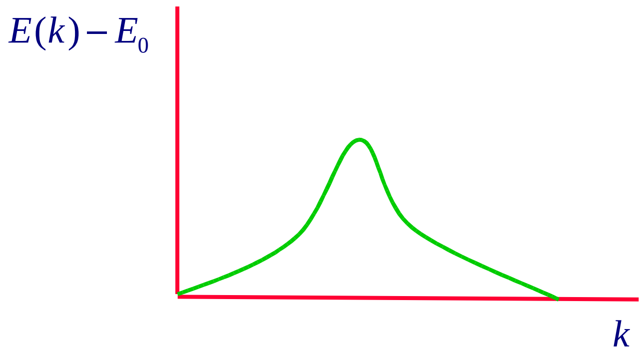
(Porras, Verstraete, Cirac, in preparation)

- *Imposing* $|\Psi\rangle = \sum_{i_1,\ldots,i_N=0}^{1} \mathrm{Tr}\left(A_1^{i_1} A_2^{i_2} \ldots A_N^{i_N}\right) | i_1,\ldots,i_N\rangle$ *we will not get a TI state.*

- *We can impose:* $|\Psi\rangle = \sum_{n=1}^{N} \mathrm{T}^n \sum_{i_1,\ldots,i_N=0}^{1} \mathrm{Tr}\left(A_1^{i_1} A_2^{i_2} \ldots A_N^{i_N}\right) | i_1,\ldots,i_N\rangle$

- *We can obtain excitations with a given momentum by choosing:*

$$|\Psi_k\rangle = \sum_{n=1}^{N} \mathrm{T}^n e^{ikn/N} \sum_{i_1,\ldots,i_N=0}^{1} \mathrm{Tr}\left(A_1^{i_1} A_2^{i_2} \ldots A_N^{i_N}\right) | i_1,\ldots,i_N\rangle$$



- *We can also obtain excitations for k=0 imposing* $\langle \Psi | \Psi_0 \rangle = 0$

4. Optimal dimensional reduction

- *We derived an algorithm to determine the best approximation by a PEPS.*
- *Given* Ψ *find the PEPS,* Ψ_D*, with fixed D for which* $\left\| \Psi - \Psi_D \right\|$ *is minimal*

Idea:

- *Fix all matrices A at all locations except for one at k.*

- *Find the A's at the k-th location by minimizing* $\left\| \Psi - \Psi_D \right\|$

Note $\left\| \Psi - \Psi_D \right\|^2 = c + \langle \Psi_D | \Psi_D \rangle - \langle \Psi_D | \Psi \rangle - \langle \Psi | \Psi_D \rangle$

thus we have to solve $M\,x = b$

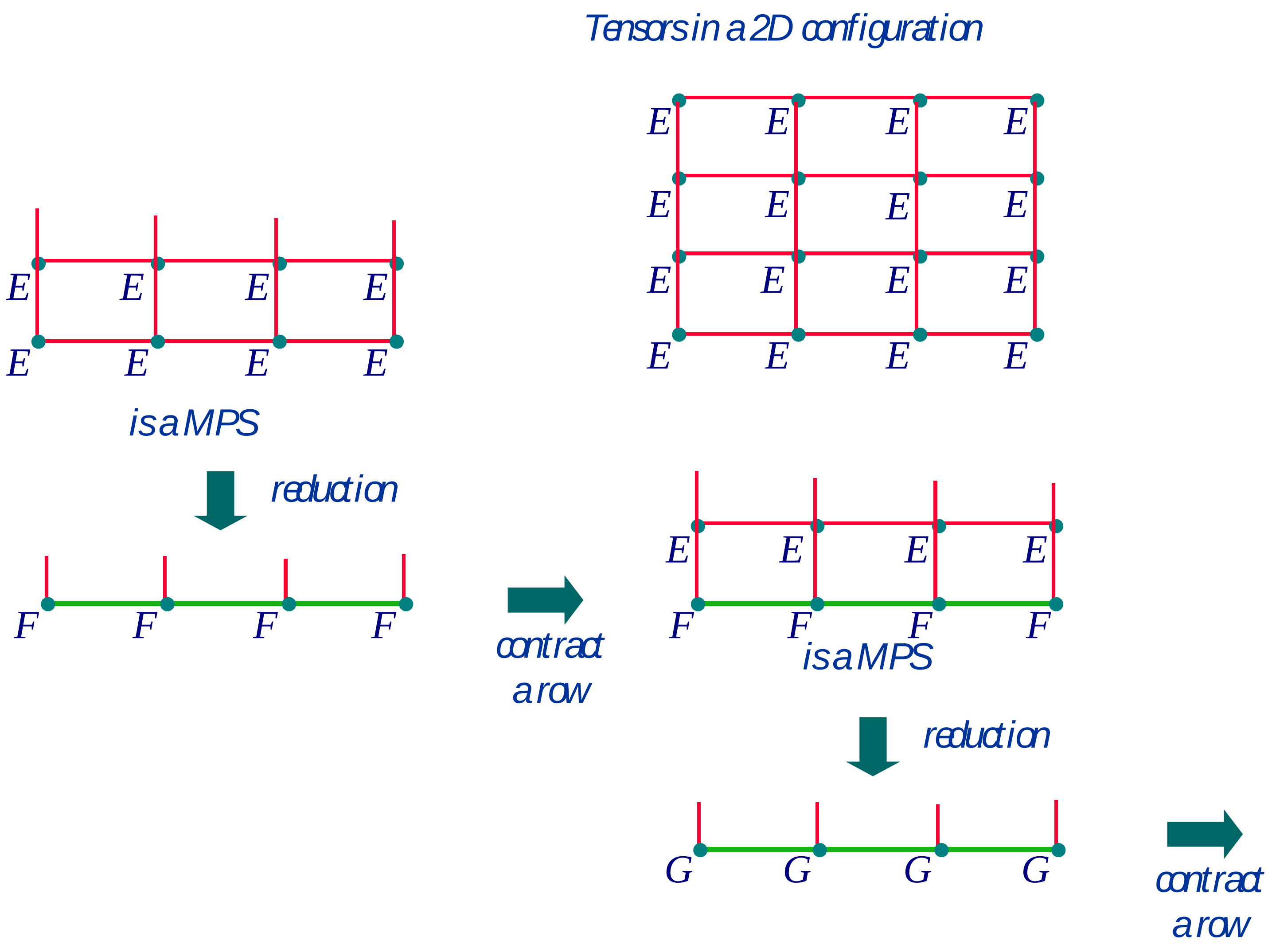
- *Iterate:*

In particular: *If* Ψ *is itself a MPS or a superposition of MPS, this is very efficient.*

Optimal dimensional reduction:

Given $\Psi_{D'}$ *we can find the optimal* Ψ_D *with minimal distance and* $D < D'$.

Application I: contracting tensors



Contracting tensors: Applications

1) Correlation functions in 2 and higher dimensions:

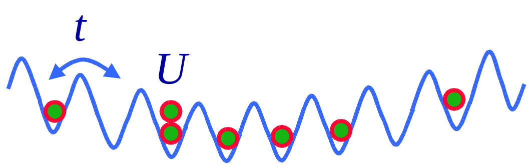
2) Classical partition function in 2 or higher dimensions:

3) Finite temperature in 1D:

- Finite
- Inhomogeneous.

(equivalent to evaluating the partition functioin for a classical model in 2D)

Example: Bose Gas in an optical lattice



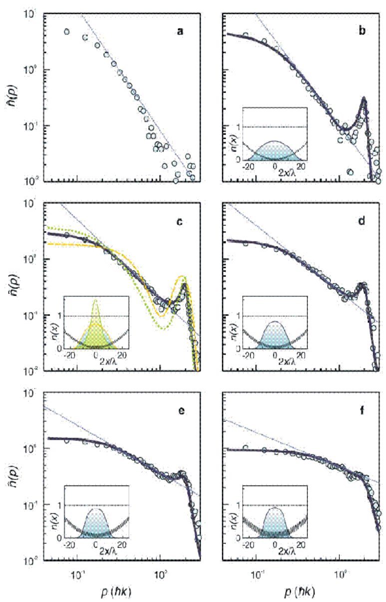
$U < \infty$

$T > 0$

Murg, Verstraete, JIC in preparation

$U \rightarrow \infty$

$T \rightarrow 0$



Tonks gas

Paredes et al, Nature 2004.

DMRG calculations

Schollwöck et al PRL 2004.

Application 2: time evolution

δt $\quad e^{-iH\delta t} \approx 1 - iH\delta t$

Optimal dimensional reduction

δt $\quad e^{-iH\delta t} \approx 1 - iH\delta t$

Optimal dimensional reduction

As compared to the method developed by G. Vidal (see also White, Schollwöck and coll):

- *Is variational (i.e., optimal) although may be slower.*
- *Works for arbitrary interactions.*
- *Works for periodic boundary conditions.*

Time evolution: Applications

1) Finite temperature:

Determine the time evolution in imaginary time:

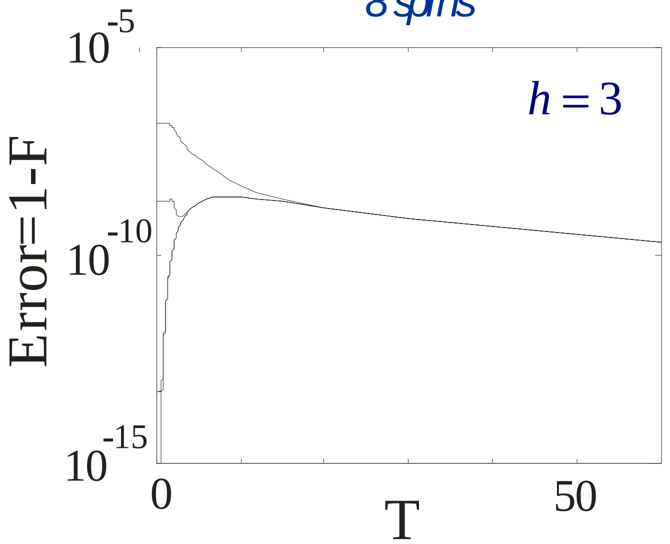
$$\rho(0) = 1 \rightarrow \rho(T) = \underbrace{e^{-\beta H/2}}_{e^{-\beta H/2M} e^{-\beta H/2M} \ldots e^{-\beta H/2M}} 1 e^{-\beta H/2} = e^{-\beta H}$$

Verstraete, Porras, and Cirac, PRL 2004: Use purification and time optimal.
Vidal and Zwolek, PRL 2004: Extension of G. Vidal's method
treat ρ as a vector and do time evolution.

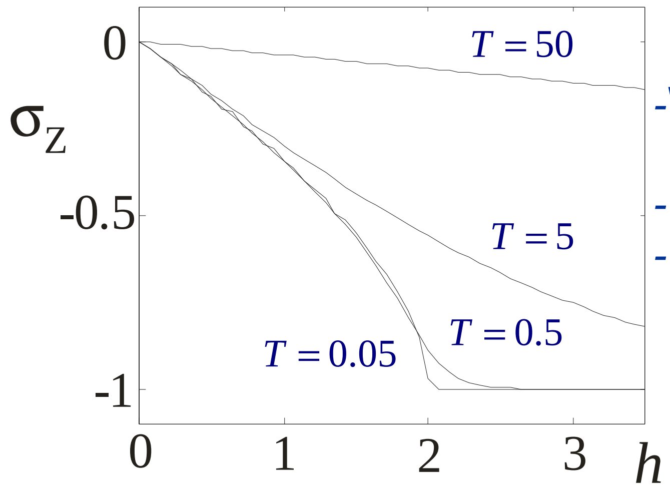
Illustration:

$$H = \sum_k \left(\sigma_x^k \sigma_x^{k+1} + \sigma_y^k \sigma_y^{k+1} \right) + h \sum_k \sigma_x^k$$

8 spins



60 spins



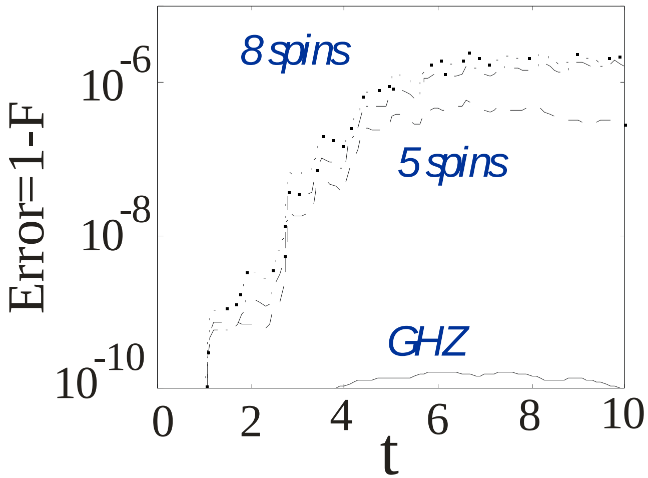
- *Valid for inhomogeneous systems.*
- *For T=0 recovers DMRG.*
- *More precise.*

2) Decoherence:

$$\frac{d}{dt}\rho = -i[H,\rho] + L\rho$$ *Master equation*

$$H = \sum_k \left(\sigma_x^k \sigma_x^{k+1} + \sigma_y^k \sigma_y^{k+1}\right) + h\sum_k \sigma_x^k$$

$$L\rho = \gamma \sum_k (\sigma_z^k \rho \sigma_z^k - \rho)$$



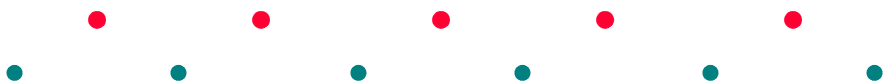
3) Spin glasses:

$$H = \sum_k J_k \sigma_z^k \sigma_z^{k+1} + h \sum_k \sigma_x^k$$

where $J_k = \pm 1$

we want to determine averaged quantities over all realizations.

Idea: consider the system



$$H = \sum_k s_z^k \sigma_z^k \sigma_z^{k+1} + h \sum_k \sigma_x^k$$

- *Evolution:*

$$e^{-iHt} |\Psi_0\rangle \left(|0\rangle + |1\rangle \right)^{\otimes N} = \sum_{s_1,\ldots,s_N=0}^{1} |s_1,\ldots,s_N\rangle e^{-iH_s t} |\Psi_0\rangle$$

- *Expectation values:*

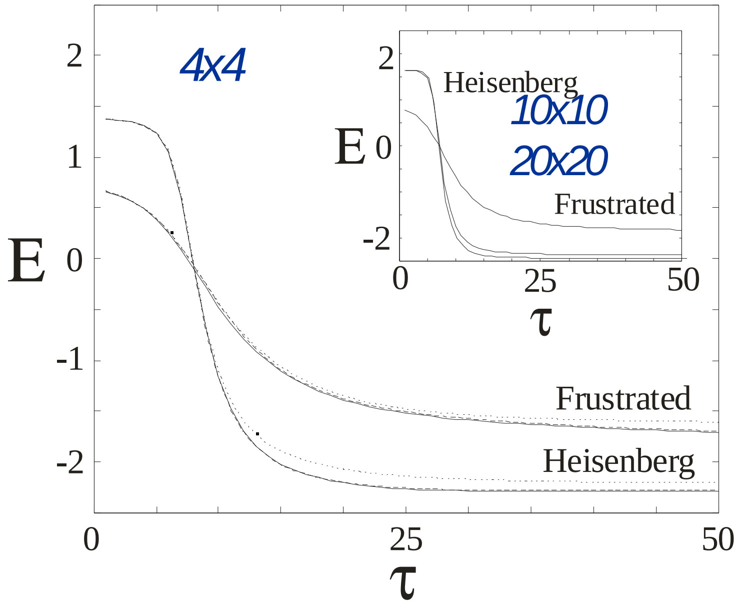
$$\langle A \otimes 1 \rangle = \sum_{s_1,\ldots,s_N=0}^{1} \langle \Psi_0 | e^{-iH_s t} A e^{-iH_s t} | \Psi_0 \rangle = \langle\langle A \rangle\rangle$$

- *Adiabatic algorithms* → *Ground state properties.*
- *Other initial states* → *Correlated glasses.*

Contracting tensors + Time evolution: 2D systems

2D Systems:

$$H = \sum_{\langle k,j \rangle} \left(\sigma_x^k \sigma_x^j + \sigma_y^k \sigma_y^j + \sigma_z^k \sigma_z^j \right)$$

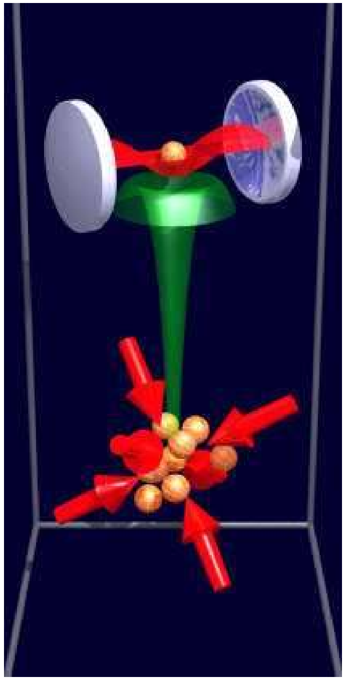


5. PEPS in Quantum Optics

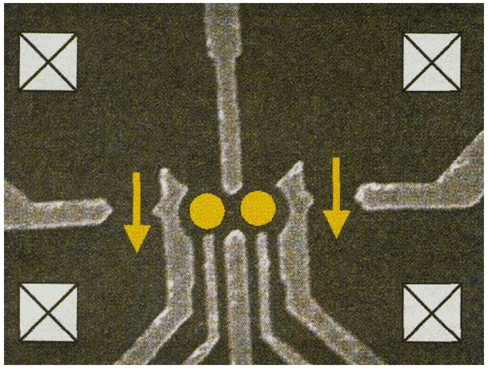
(C. Schön, E. Solano, M. Wolf, I. Cirac, in preparation)

Photon generators:

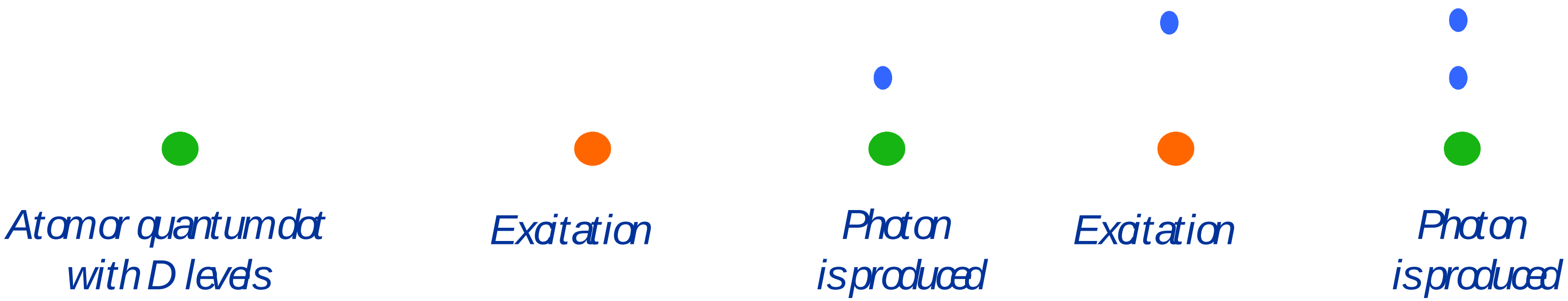
Cavity QED
Rempe, Kimble, Walther



Quantum dots
Yamamoto, Finley, Imamouglu, etc



General scheme:

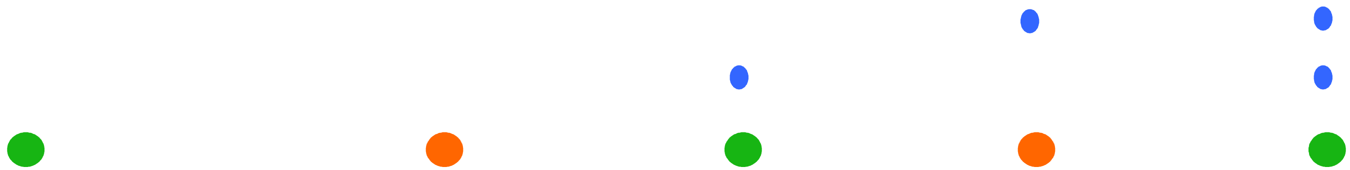


What kind of states can this system produce?

For N photons, the Hilbert space has dimension 2^N

We have access to DN parameters

General scheme:



$$\sum_{\alpha=1}^{D}\sum_{i_1=0}^{1} A_{\alpha}^{i_1}\,|\alpha\rangle\,|i_1\rangle$$

$$\sum_{\alpha,\beta=1}^{D}\sum_{i_1=0}^{1} A_{\alpha}^{i_1}A_{\alpha\beta}^{i_2}\,|\beta\rangle\,|i_1\rangle\,|i_2\rangle$$

In general: $$|\Psi\rangle = \sum_{i_1,\dots,i_N=0}^{1} \mathrm{Tr}\left(A_1^{i_1}A_2^{i_2}\dots A_N^{i_N}\right)|i_1,\dots,i_N\rangle$$

The generated states are 1D PEPS with D.

Other activities on QI at MPQ

Localizable entanglement

F. Verstraete, M. Popp, M. Martin-Delgado

Entanglement and SSRules

F. Verstraete, N. Schuch

Gaussian states and channels

M. Wolf and N. Schuch

Q. Computing with global operations

K. Vollbrecht

Entanglement flow

T. Cubitt and F. Verstraete

Physical implementations

- *Trapped ions*
  J. Garcia-Ripoll, D. Porras
- *Optical lattices*
  K. Vollbrecht, E. Solano
- *Quantum dots*
  H. Chist, B. Paredes
- *Atomic ensembles*
  K. Hammerer

Entanglement detection — *G. Toth*

Quantum Cryptography — *F. Grossans*

Channel capacities — *M. Wolf, K. Vollbrecht*

References

Quantum computation and error correction: *2D systems:*	*F. Verstraete*
Problems with periodic boundary conditions: *Excitations:*	*F. Verstraete, D. Porras*
Finite temperature:	*F. Verstraete,* *J.J. Garcia-Ripoll,* *V. Murg*
Spin glasses:	*F. Verstraete, B. Paredes*
Quantum optical systems:	*M. Wolf,* *C. Schön, E. Solano*