

# DMRG 101: Introduction to Theory and Practice

When: August 12, 2016

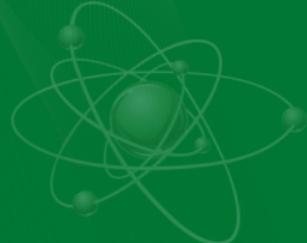
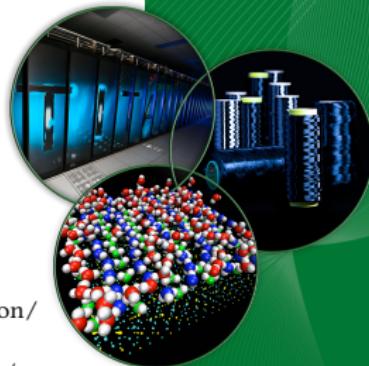
Where: ORNL, Oak Ridge, TN, USA

Attendance is free but registration is required

<https://public.ornl.gov/conferences/cnms2016/registration/>

<https://public.ornl.gov/conferences/cnms2016/workshop4/>

Organizers: G. Alvarez and A. Nocera



# DMRG 101: Introduction to Theory and Practice

This workshop will present the basics of the Density Matrix Renormalization Group algorithm. The Density Matrix Renormalization Group (DMRG) is one of the most powerful numerical techniques for studying many-body systems. It was developed in 1992 by Steven R. White at the University of California in Irvine to overcome the problems arising in the application of the Numerical Renormalization Group to quantum lattice many-body systems such as the Hubbard model of strongly correlated electrons. Since then the approach has been extended to a great variety of problems in all fields of physics and to quantum chemistry.

We will start with an introduction of the algorithm, and a brief explanation of the foundations. There will be an overview of the literature for those interested in a more rigorous theoretical treatment. Most of focus will then turn to the practice of the algorithm using the DMRG++ application, which is a free and open source implementation of the DMRG algorithm.

The workshop will explain how to simulate the Heisenberg model, the Hubbard model and the t-J model, starting from the calculation of energies, followed by static observables, such as densities, and charge and spin correlations. We will end with a brief overview of applications for time evolution, temperature, and spectral functions.

*Needed Material:* Participants need to bring a computer that can compile C++ programs, with the gcc compiler or the clang compiler. The LAPACK and BLAS libraries, and the computer programs perl, make and git are needed as well.

## Tutorial Aims

At the end of this tutorial,

- ① you will have understood the correlated electron problem in condensed matter,
- ② you will have understood the solution to that problem based on the DMRG.
- ③ By following through the worked exercises during the tutorial, you will have a working knowledge of ground state DMRG applied to models of quantum spins, and correlated electrons.
- ④ You will be ready to expand your knowledge of DMRG into time evolution, temperature, and dynamics.
- ⑤ Finally, you will know enough to be able to follow current research in the area of DMRG, and understand the current race to solve the two-dimensional problem.

# Agenda

## 1 DMRG Basics

- 09:00–09:30 The Problem
- 09:30–10:00 The Density Matrix
- 10:00–10:45 DMRG Algorithm
- 10:45–11:00 Break

## 2 Ground State DMRG

- 11:00–12:00 Models and Geometries
- 12:00–01:15 Lunch Break
- 01:15–02:30 Exercises

## 3 Time, Temperature, Dynamics

- 02:30–03:00 Time
- 3:00–3:30 Temperature
- 3:30–4:00 Dynamics
- 4:00–4:30 Break

## 4 Beyond DMRG

# Navigation Slide

Skip software slides, and jump to 13

## Downloading the computer codes

Although not required, you are encouraged to prepare for the tutorial by downloading the computer codes as explained below. You are also encouraged to test compilation as explained below.

### Computer Code Licenses

The computer codes mentioned in this tutorial are all free and open source, and their licenses are available in the file LICENSE in the source code of each.

### This Tutorial License

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<https://creativecommons.org/licenses/by-nc-sa/4.0/>

# Downloading the computer codes

## Downloading GNUPG Keys

```
git clone https://github.com/g1257/SecurityPack  
cd SecurityPack/keys  
gpg --with-fingerprint gz1-master-key.txt
```

### Check Fingerprint

Key fingerprint = C374 4A1F 30DE 79AA BF1B 7A33 CBB8 FD57 167A 6E04

```
gpg --import gz1-master-key.txt  
gpg --edit-key gz1-master-key.txt
```

# Downloading the computer codes

## Downloading GNUPG Keys (continued)

fpr

C374 4A1F 30DE 79AA BF1B 7A33 CBB8 FD57 167A 6E04

After verifying the fingerprint, you can either sign my key with your key or trust

(ultimate trust)

Now you may import the code signing key,  
gpg --import gz1-code-signing-key.txt  
gpg --check-sigs

Make sure key 805ABC35 is signed by 167A6E04, you should see  
sig! 0xCBB8FD57167A6E04

More details at <https://web.ornl.gov/~gz1/keys.html>

## Downloading the computer codes

```
mkdir mydirectory/  
cd mydirectory/  
git clone https://github.com/g1257/PsimagLite  
git clone https://github.com/g1257/LanczosPlusPlus  
git clone https://github.com/g1257/dmrgpp  
git clone https://github.com/g1257/FreeFermions  
git clone https://github.com/g1257/BetheAnsatz
```

This last repo will be available on tutorial's day,  
git clone https://github.com/g1257/dmrg101

# Verifying Codes and Compiling them

## Verifying codes

```
cd PsimagLite/lib  
git pull --ff-only --verify-signatures  
git log --show-signature -1  
gpg: Good signature from “Gonzalo Alvarez (Code Signing Only) (Code  
Signing Key) <gz1@ornl.gov>”
```

Now you are ready to compile,

```
perl configure.pl  
make
```

# Verifying Codes and Compiling them

(continued)

Proceed like before for the rest of the codes.

```
cd ../../LanczosPlusPlus/src  
git pull --ff-only --verify-signatures  
git log --show-signature -1
```

Make sure you get a *Good signature* and then compile with

```
perl configure.pl  
make
```

DMRG++ can take half an hour to compile

```
cd ../../dmrgpp/src  
git pull --ff-only --verify-signatures  
git log --show-signature -1  
perl configure.pl  
make
```

# Verifying Codes and Compiling them

(continued)

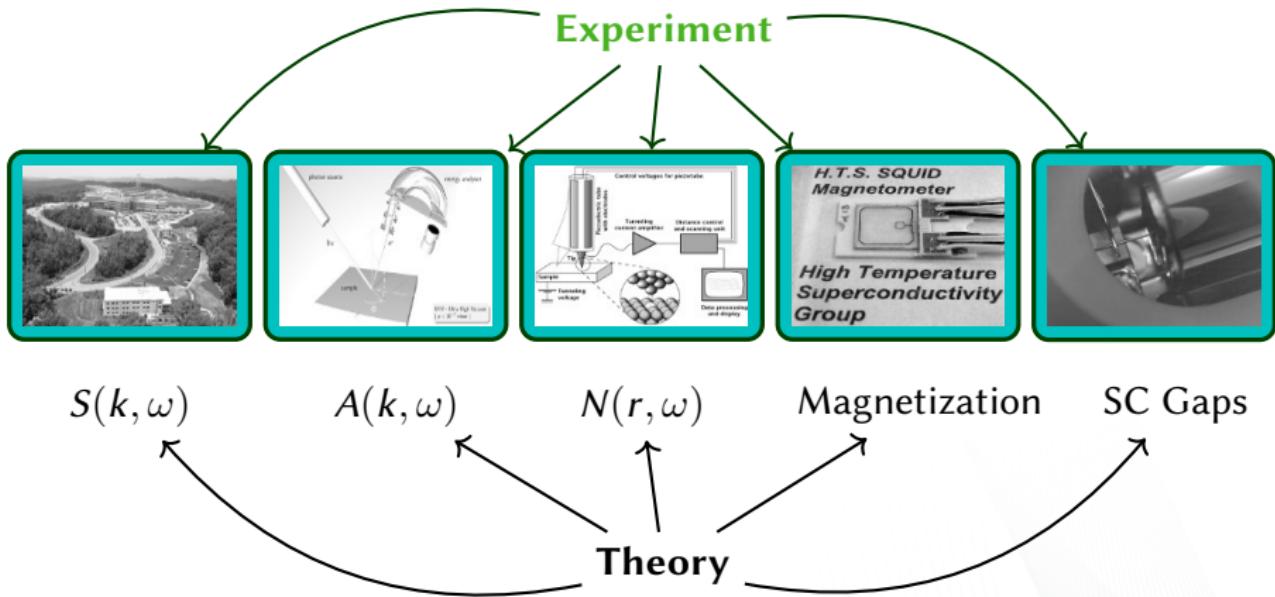
```
cd ../../BetheAnsatz/src  
git pull --ff-only --verify-signatures  
git log --show-signature -1  
make
```

Please write to G. Alvarez (gz1 at ornl dot gov) if there are problems with downloading, or verifying, or compiling the computer codes.

Optional return to 34



# Experiment and Theory



# First Quantization of Condensed Matter

$$H = H_n + H_{1e} + H_{e-e}, \quad (1)$$

where

$$H_n = \sum_{j \in \mathcal{A}} \frac{P_j^2}{2M_j} + \frac{e_2}{2} \sum_{j \neq j' \in \mathcal{A}} \frac{Z_j Z_{j'}}{|\vec{R}_j - \vec{R}_{j'}|}, \quad (2)$$

$$H_{1e} = \sum_{i \in \mathcal{E}} \frac{p_i^2}{2m} - e^2 \sum_{i \in \mathcal{E}, j \in \mathcal{A}} \frac{Z_j}{|\vec{r}_i - \vec{R}_j|}, \quad (3)$$

$$H_{e-e} = \frac{e_2}{2} \sum_{i \neq i' \in \mathcal{E}} \frac{1}{|\vec{r}_i - \vec{r}_{i'}|}. \quad (4)$$

## What's the problem?

The problem is to solve the Schrödinger equation  $H\psi = E\psi$ , where  $E$  is the lowest or ground state energy.

## Atoms and Electrons

Efficient solution exists if  $H_{e-e}$  is ignored or approximated: Local Density Approximation or LDA. LDA works because electrons in Matter are often weakly correlated and easy to study....But not always.

Electrons in many materials are strongly correlated and difficult to study. For example,

- superconductors,
- magnetic materials,
- quantum dots, and
- transition metal oxides.

They are also technologically useful.

# How do electron correlations cause functionality?

**Answer:** By having different phases, usually close in energy.

These phases present one order that can be easily (energetically speaking) turned into another.\*

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\* See  Dagotto, 2005.

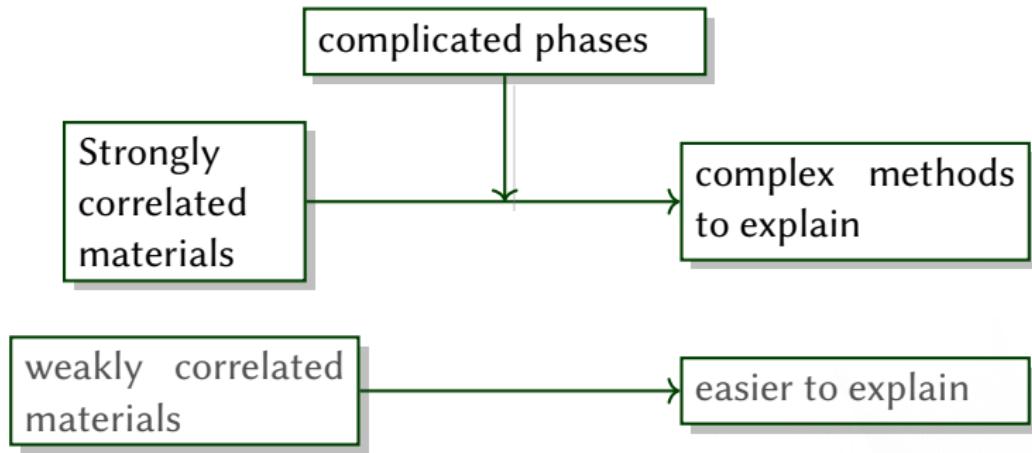
# What causes the energetically-close phases?

**Answer:** The competition between different tendencies, such as...

- FM vs. AFM in spin,
- orbital-order vs. orbital-disorder in orbital,
- order vs. disorder in lattice distortions or phonons,
- etc.

This competition originates in the strong **correlation** between electrons.

# What causes the energetically-close phases?



# Why are these materials costly to study?

**Answer:** Because of  $H_{e-e}$  the “standard one-electron model” of metals breaks down, and LDA cannot be used

Therefore, an **accurate** approach to study strongly correlated materials is needed.

And accurate approaches are computationally **costly**.

# Condensed Matter in Second Quantization

## The Hilbert Space

$c_{i\uparrow}^\dagger$  creates an electron with spin  $\uparrow$  on site  $i$ , whereas  $c_{i\uparrow}$  destroys it.

$$c_{i\uparrow}^\dagger |0\rangle = |\cdots \uparrow \cdots\rangle$$

Heisenberg spin 1/2  $\vec{q} = \{1, 0\}$

t-J  $\vec{q} = \{(1, 1), (1, 0), (0, 0)\}$

Hubbard  $\vec{q} = \{(1, 1), (1, 0), (0, 0), (1, 2)\}$

And many more<sup>1</sup>

<sup>1</sup> Spalek and Oleś, 1977, Hubbard, 1963, Hubbard, 1964

# Condensed Matter in Second Quantization

## The Hamiltonian

$$H = \sum_{i,j} \langle i | \hat{K} | j \rangle c_i^\dagger c_j + \sum_{i,j,k,l} \langle ij | \hat{H}_{e-e} | kl \rangle c_i^\dagger c_j^\dagger c_k c_l$$

### What's the problem?

Finding lowest eigenvalue  $E$  and lowest eigenvector  $v$  such that  $Hv = Ev$ .

### Example: Hubbard model 2 sites



What are the possible quantum numbers ( $N_\uparrow, N_\downarrow$ )? See 23.  
How many states are there with a given ( $N_\uparrow, N_\downarrow$ )?  $C_{N_\uparrow}^N C_{N_\downarrow}^N$ .  
Can we assign a single number to each pair? Yes.

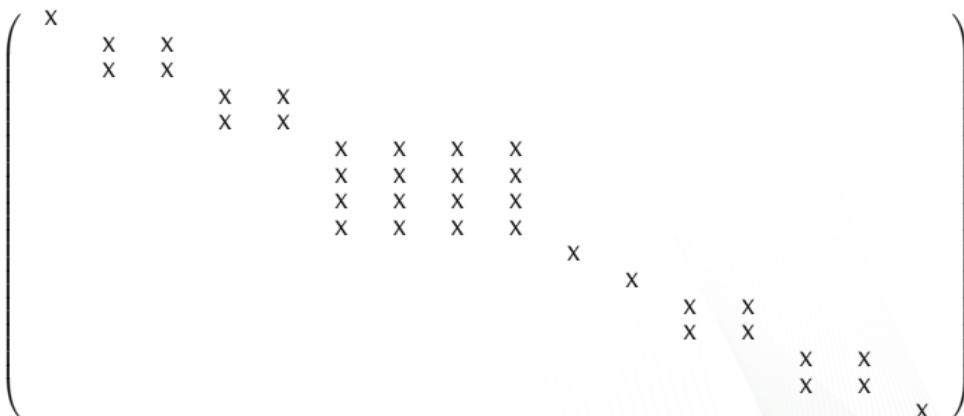
# Condensed Matter in Second Quantization

## Symmetry Sectors and Hamiltonian Blocking

Example: Hubbard model 2 sites: There are  $2^4 = 16$  states



$N_\uparrow$	$N_\downarrow$	Size
0	0	1
1	0	2
0	1	2
1	1	4
2	0	1
0	2	1
2	1	2
1	2	2
2	2	1



$$2^4 = 16 = 1 + 2 + 2 + 4 + 1 + 1 + 2 + 2 + 1$$

# Condensed Matter in Second Quantization

What's the Problem?

## Summary

You have understood the Hilbert space of second quantization, the Hamiltonian of second quantization, the local symmetries of the Hamiltonian, and the blocking of the Hamiltonian

The problem is to solve the Schrödinger equation. In second quantization it implies finding lowest eigenvalue  $E$  and lowest eigenvector  $v$  such that

$$Hv = Ev$$

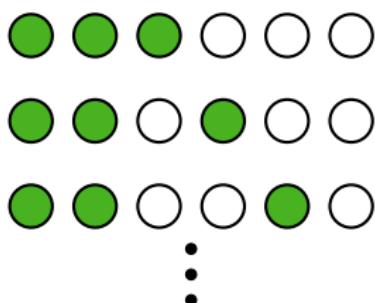
Then  $v$  can be used to compute observables  $O$  with  $v^T O v$ .

# Condensed Matter in Second Quantization

The Problem is Exponential

Example: Heisenberg model, 6 sites,

$$S^z = 0: C_3^6 = 20 \text{ states}$$



For large  $N$  we have Stirling's approximation

$$N! \rightarrow \sqrt{2\pi N} \left(\frac{N}{e}\right)^N$$

Storage would also be exponential

Even if we had the solution, we couldn't store it, much less use it. We need not just to solve the problem, but to find an efficient representation as well.



## What does exponential *really* mean?

- Assume  $N_f$  “flavors” or orbitals (including spin),  $N$  sites
- Assume no symmetries (won’t change the argument much)
- Then complexity is  $2^{N \times N_f}$ .
- Assume a more or less realistic problem:  
 $N_f = 10, N = 10$
- Exact diagonalization would take  $\approx 10^6$  billion years to complete
- Problem not even in NP.... See 109.
- We need an efficient representation not just a solution.

# The Reduced Density Matrix

1

## DMRG Basics

- 09:00–09:30 The Problem
- **09:30–10:00 The Density Matrix**
- 10:00–10:45 DMRG Algorithm
- 10:45–11:00 Break

2

## Ground State DMRG

3

## Time, Temperature, Dynamics

4

## Beyond DMRG

## The Heisenberg model spin 1/2

$S_i^+$  flips an electron from down ( $m = -1/2$ , empty circles) to up ( $m = 1/2$ , filled circles) if it was down, or yields  $\emptyset$ , the zero of the Hilbert space.  $S_i^-$  does the opposite.  $S_i^z$  is diagonal multiplied by  $m_i$ .

  $m = 1/2$

  $m = -1/2$

$$S^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad S^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

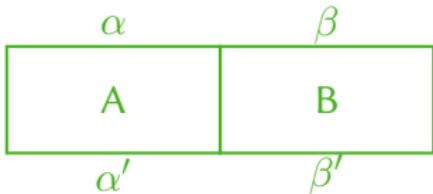
### Example: 4 sites



### Example: 4 sites, $S^z = 0$ symmetry sector



# The Reduced Density Matrix



$$|\psi\rangle = \sum_{\alpha,\beta} \psi_{\alpha,\beta} |\alpha\rangle \otimes |\beta\rangle$$

$$\rho^S = W^\dagger D W, \bar{A} = W A W^\dagger$$

$\{|\alpha\rangle\}$  basis of  $A$ ,  $\{|\beta\rangle\}$  basis of  $B$ ,  $\{|\alpha\rangle \otimes |\beta\rangle\}$  basis of  $A \cup B$ .

$$\begin{aligned}
 \langle \psi | A \otimes I | \psi \rangle &= \sum_{\alpha,\alpha',\beta} \psi_{\alpha,\beta}^* A_{\alpha,\alpha'} \psi_{\alpha',\beta} = \sum_{\alpha,\alpha'} A_{\alpha,\alpha'} \sum_{\beta} \psi_{\alpha,\beta}^* \psi_{\alpha',\beta} \\
 &= \sum_{\alpha,\alpha'} A_{\alpha,\alpha'} \rho_{\alpha',\alpha}^S = \text{Tr}(A \rho^S) = \text{Tr}(A W^\dagger D W) = \text{Tr}(W A W^\dagger D) = \\
 &= \sum_{\alpha} \bar{A}_{\alpha,\alpha} d_{\alpha} = \sum_{\alpha < m} \bar{A}_{\alpha,\alpha} d_{\alpha} + E(m), \text{ where the error } E(m) \text{ is}
 \end{aligned}$$

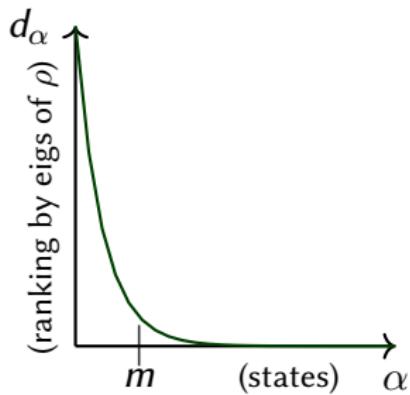
$$E(m) = \sum_{\alpha >= m} \bar{A}_{\alpha,\alpha} d_{\alpha} \leq \bar{A}_{\max} \sum_{\alpha >= m} d_{\alpha}.$$

# The Eigenvalues of the Density Matrix



$$|\psi\rangle = \sum_{\alpha,\beta} \psi_{\alpha,\beta} |\alpha\rangle \otimes |\beta\rangle$$

$$\rho^S = W^\dagger D W, \bar{A} = W A W^\dagger$$



Recall definition of reduced density matrix of A with respect to B:

$$\rho_{\alpha,\alpha'}^A \equiv \sum_{\beta} \psi_{\alpha,\beta}^* \psi_{\alpha',\beta}$$

Notation

$A \equiv S \equiv$  left block  $\equiv$  “the system”

$B \equiv E \equiv$  right block  $\equiv$  “the environ”

$A \cup B \equiv$  “superblock”

# Properties of the Density Matrix

## Exercise 1

Prove that the reduced density matrix is Hermitian, positive-semidefinite, and that the sum of its eigenvalues is 1. Prove also that if  $\lambda$  is an eigenvalue of the reduced density matrix, then  $0 \leq \lambda \leq 1$ . *Hint:* Use the definition of  $\rho$ , and that  $\sum_{\alpha,\beta} |\psi_{\alpha,\beta}|^2 = 1$ , that is, that  $\psi$  is normalized.

## Exercise 2      Pure State

If  $\psi_{\alpha,\beta} = v_\alpha w_\beta$  for some normalized vectors  $v$  and  $w$ , then find the eigenvalues of the reduced density matrix of  $|\psi\rangle$ .

## Exercise 3      Maximally Entangled State

Let the blocks  $A$  and  $B$  be identical, each with Hilbert space of dimension  $n > 0$ . If  $\psi_{\alpha,\beta} = \delta_{\alpha,\beta}/\sqrt{n}$ , then find the eigenvalues of the reduced density matrix of  $|\psi\rangle$ .

# Reduced Density Matrix (continued)

## Exercise 4

Let the blocks  $A$  and  $B$  be identical, each with Hilbert space of the Heisenberg model for spin  $s$ . If  $\psi_{\alpha,\beta} = c(1 - \delta_{\alpha,\beta})$ , where  $c$  normalizes the state, then write down the state  $|\psi\rangle$  for  $s = 1/2$  and for  $s = 1$ .

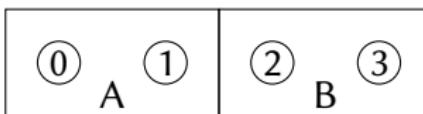
## Exercise 5

Let the blocks  $A$  and  $B$  be identical, each with Hilbert space of dimension  $n > 0$ . If  $\psi_{\alpha,\beta} = c(1 - \delta_{\alpha,\beta})$ , where  $c$  normalizes the state, then find the eigenvalues of the reduced density matrix of  $|\psi\rangle$  for  $n = 2$  and for  $n = 3$ .

# Downloading the computer codes

Please see slide 6.

## Example: 4-site Heisenberg



```
cp ../../dmrg101/inputs/tutorial2016n*.inp.  
Please see tutorial2016n0.inp and DMRG++ manual.
```

TotalNumberOfSites=4

Model=Heisenberg

HeisenbergTwiceS=1

Connectors 1 1.0

GeometryOptions=ConstantValues

Connectors 1 1.0

TargetElectronsTotal=4

TargetSzPlusConst=2

Model

$S = 1/2$  Heisenberg

$J_{\pm} = 1.0$ , 1 Connector given

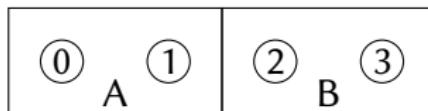
Spacially constant connectors

$J_z = 1.0$

FIXME

# of electrons with  $m = 1/2$

## Example: 4-site Heisenberg



```
./lanczos -f tutorial2016n0.inp
Energy=-1.616
./lanczos -f tutorial2016n0.inp -c sz
0.25 -0.228 0.061 -0.083
...
...
```

$$A = S_0^z S_1^z, \langle S_0^z S_1^z \rangle = -0.228$$

```
./lanczos -f tutorial2016n0.inp -r 2
```

---

<sup>1</sup>All numbers rounded here and elsewhere in these slides.

## 4-site Heisenberg: The Reduced Density Matrix

RDM

0.022	0	0	0
0	0.478	-0.456	0
0	-0.456	0.478	0
0	0	0	0.022

Eigenvector W of RDM

0	1	0	0
$-1/\sqrt{2}$	0	0	$-1/\sqrt{2}$
$-1/\sqrt{2}$	0	0	$1/\sqrt{2}$
-0	0	1	0

$$A = S_0^z S_1^z$$

Eigs.: 0.022 (3x), 0.933

$$A = S_0^z S_1^z$$

$$2S_0^z = \text{diag}(1, 1, -1, -1)$$

$$2S_1^z = \text{diag}(1, -1, 1, -1)$$

$$4S_0^z S_1^z = \text{diag}(1, -1, -1, 1)$$

$$W^\dagger S_0^z S_1^z W$$

$$\begin{matrix} -0.25 & \dots & \dots & \dots \end{matrix}$$

$$\begin{matrix} \dots & 0.25 & \dots & \dots \end{matrix}$$

$$\begin{matrix} \dots & \dots & 0.25 & \dots \end{matrix}$$

$$\begin{matrix} \dots & \dots & \dots & -0.25 \end{matrix}$$

## Truncation

Keeping all states we get<sup>2</sup>

$$\langle A \rangle = (-0.25)d_0 + 0.25d_1 + 0.25d_2 - 0.25d_3 = -0.228,$$

$d_0 = d_1 = d_2 = 0.022$  and  $d_3 = 0.933$ , and the *Error*( $m = 4$ ) = 0.

Keeping only one state we get

$$\langle A \rangle \approx -0.25d_3 = -0.233.$$

And the error is

$$\text{Error}(m = 1) = (-0.25)d_0 + 0.25d_1 + 0.25d_2 = 0.005,$$

---

<sup>2</sup>Warning: Truncated numbers throughout.

## Exercises

### Exercise 6

Plot RDM eigenvalues for a 12-site Heisenberg chain.

```
lanczos -f tutorial2016n1.inp -r 6 &> out.txt
```

### Exercise 7

For the Hubbard model, we saw that in symmetry sector ( $N_\uparrow, N_\downarrow$ ) there are  $C_{N_\uparrow}^N C_{N_\downarrow}^N$  states. How many states are there in each symmetry sector of the Heisenberg  $s = 1/2$  model?

### Exercise 8

How many states are there in each symmetry sector of the t-J model?

### \* Exercise 9

How many states are there in each symmetry sector of the Heisenberg model for general  $s$ ?

# DMRG Algorithm

1

## DMRG Basics

- 09:00–09:30 The Problem
- 09:30–10:00 The Density Matrix
- **10:00–10:45 DMRG Algorithm**
- 10:45–11:00 Break

2

## Ground State DMRG

3

## Time, Temperature, Dynamics

4

## Beyond DMRG

# Renormalization Group

## Motivation to DMRG

We don't have  $\psi$ !

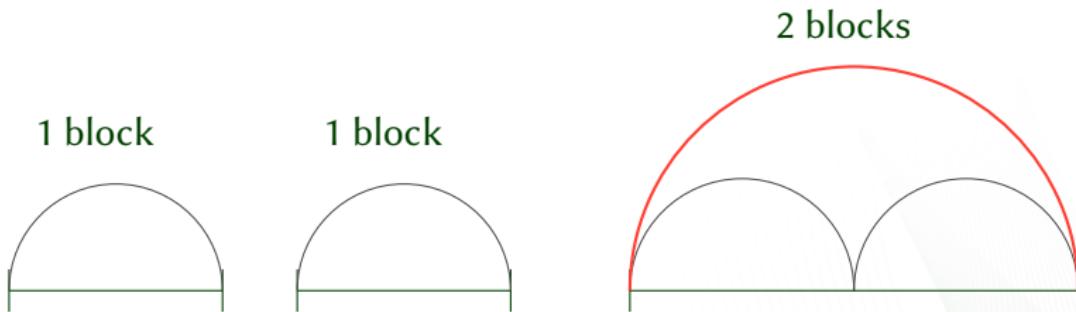
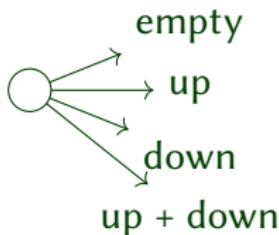
To compute the reduced density matrix of a large system, we need the ground state vector  $\psi_{\alpha,\beta}$  of a large system...which we don't have...if we had it we had solved the problem!

We need to build  $\psi$  in parts

We need to build the large system in parts. We start with a small part, truncate it using the reduced density matrix, grow it by one site, truncate it again using reduced density matrix, grow it by one site, ...

# Renormalization Group

Naïve approach doesn't work



More details in White and Noack, 1992.

# Density Matrix Renormalization Group

- For 1D systems exponential problem can be avoided.
- Algorithm: “Density Matrix Renormalization Group”

 White, 1992, White, 1993



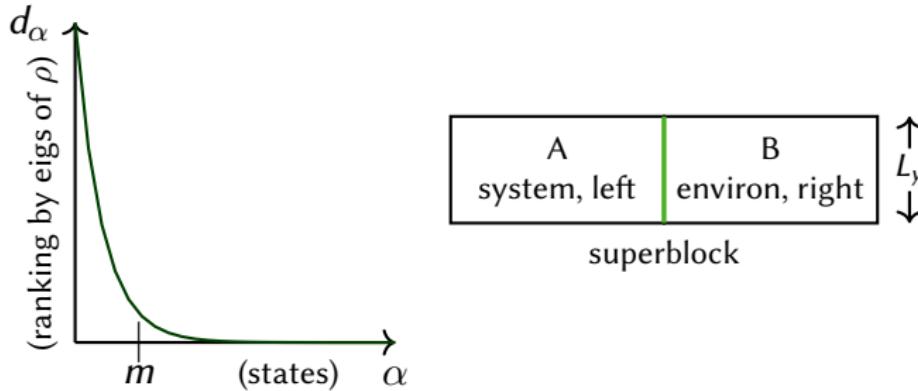
system

environment

- Discard (an exponential number of) states. Keep  $m$  states in Hilbert space at all times.
- Controlled error, exponentially decaying with  $m$  for most 1D systems.

# When does the DMRG work best?

**Answer:** When there's low entanglement



How much entanglement between A and B?

A: Roughly equal to the area between A and B.

1D: Entropy  $\rightarrow S \approx 1 \rightarrow \text{complexity} = \exp^S = \text{const.}$

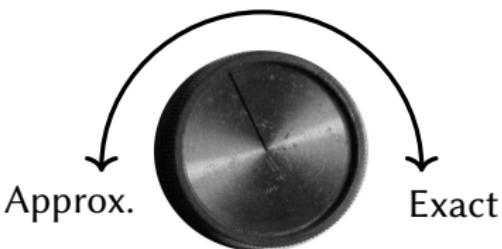
2D: Entropy  $\rightarrow S \approx L_y \rightarrow \text{complexity} = \exp^{L_y} = \text{exponential}$

For details, see Eisert et al., 2010

# Applications of the DMRG

- Spin systems quantum Heisenberg model
- Fermionic systems Hubbard, t-J models
- Quantum chemistry,  
    [book icon] White and Martin, 1999
- Polymers  
    [book icon] Lepetit and Pastor, 1997

# Only Two Methods: DMRG and Aux-QMC



Method must become exact systematically

---

Item	DMRG	QMC
Complexity	Pol. in 1D, Exp. in 2D	Pol., Exp. if SP*
Real time and freq.	Yes	Not Directly
Finite temperature	Possible	Yes
Active Research	Yes	Yes

---

\*SP stands for Sign Problem

# DMRG step by step

1  $step = 0, \mathcal{V}_R(S) \equiv \mathcal{V}(S), \mathcal{V}_R(E) \equiv \mathcal{V}(E)$ .

2

$$S' = S \cup X_{step}, \mathcal{V}(S') = \mathcal{V}_R(S) \otimes \mathcal{V}(X_{step})$$

$$E' = E \cup Y_{step}, \mathcal{V}(E') = \mathcal{V}_R(E) \otimes \mathcal{V}(Y_{step})$$

- 3 Diagonalize  $\hat{H}_{S' \cup E'}$  over  $\mathcal{V}(S') \otimes \mathcal{V}(E')$  to obtain  $\psi$
- 4 Obtain Density Matrix  $\hat{\rho}_S$  from  $\psi$
- 5 Diagonalize Density Matrix  $\hat{\rho}_S$  to obtain  $w_{\alpha,\alpha'}^S$  (similar for E)
- 6 Truncate  $w^S$  if necessary (similar for  $w^E$ )
- 7  $H^{S'}$  into  $w^{S\dagger} H^{S'} w^S$  (similar for E)
- 8  $step++, S \leftarrow S', \mathcal{V}_R(S) \leftarrow \mathcal{V}_R(S'), H_{S'} \leftarrow H_S$  (similar for E)
- 9 Goto 2

See [White, 1993](#). Implementation details in [Alvarez, 2009](#).

# The Input File

---

TotalNumberOfSites=4	
Connectors 1 1.0	$J_{\pm} = 1.0$ , 1 Connector given
GeometryOptions=ConstantValues	Spacially constant connectors
Connectors 1 1.0	$J_z = 1.0$
Model=Heisenberg	Model
HeisenbergTwiceS=1	$S = 1/2$ Heisenberg
TargetSzPlusConst=2	# of electrons with $m = 1/2$
OutputFile=tutorial2016data0.txt	
InfiniteLoopKeptStates=60	$m$ for the “infinite” loop

---

## “Infinite” DMRG



system

environment

Please compile PsimagLite if you haven't yet.

```
cd ../../dmrgpp/src
git pull
git log --show-signature -1
perl configure.pl
make
./dmrg -f tutorial2016n0.inp
grep lowest runFortutorial2016n0.cout
./dmrg -f tutorial2016n1.inp
grep lowest runFortutorial2016n1.cout
```

“Infinite” DMRG

S+E	Energy
2+2	-1.616
3+3	-3.375
4+4	-4.258
5+5	-5.142
6+6	...

## “Finite” DMRG



How do we shrink a basis? **Answer:** We just use a previously saved one.

Each vertical dashed line defines a **center of orthogonality**, and defines a Hilbert space basis, referred to as the DMRG basis at that center.

---

TotalNumberOfSites=4

Model=Heisenberg

Model

TargetSzPlusConst=2

# of electrons with  $m = 1/2$

InfiniteLoopKeptStates=60

$m$  for the “infinite” loop

FiniteLoops 4

4 Triplets of number follow

1 100 0

Go right 1, use  $m = 100$ , flag=0

---

## Two-point correlations

Compute 4-site Heisenberg correlation with DMRG

```
./dmrg -f tutorial2016n0.inp
```

Measuring post-processing:

```
./observe -f tutorial2016n0.inp '<gs|z;z|gs>'  
<gs|z;z|gs>  
4 4  
0.25 -0.228 0.061 -0.083  
0 0.25 -0.0833 0.061  
0 0 0.25 -0.228  
0 0 0 0.25
```

# Break

1

## DMRG Basics

- 09:00–09:30 The Problem
- 09:30–10:00 The Density Matrix
- 10:00–10:45 DMRG Algorithm
- 10:45–11:00 Break

2

## Ground State DMRG

3

## Time, Temperature, Dynamics

4

## Beyond DMRG

## Exercises

### Exercise 10

For a 12-site Heisenberg chain, compute the spin correlations with DMRG.

*Hint:* Use first `./dmrg -f tutorial2016n1.inp`, and then  
`./observe -f tutorial2016n1.inp '<gs|z;z|gs>'`

### Exercise 11

What's the largest  $m$  that makes sense for the case of `tutorial2016n1`?

### Exercise 12

By modifying the number of kept states  $m$  in `tutorial2016n1`, plot  $\langle S_0^z S_1^z \rangle$  vs.  $m$ . Suggested values of  $m$  are 10, 20, 40, 60 and the value of previous exercise. Do DMRG results converge to the exact value?

# The Need for Truncation

## Exercise 13

What is the largest size  $L$  that Lanczos alone can simulate in the case of the Heisenberg model spin 1/2?

Answer: 35 sites for Heisenberg  $\Rightarrow s = I \backslash S$ .

### Answer of exercise 13

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1/\sqrt{2} & 0 & 0 & -1/\sqrt{2} \\ -1/\sqrt{2} & 0 & 0 & 1/\sqrt{2} \\ 0 & 0 & 1 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 \\ -1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \end{pmatrix} \equiv w$$

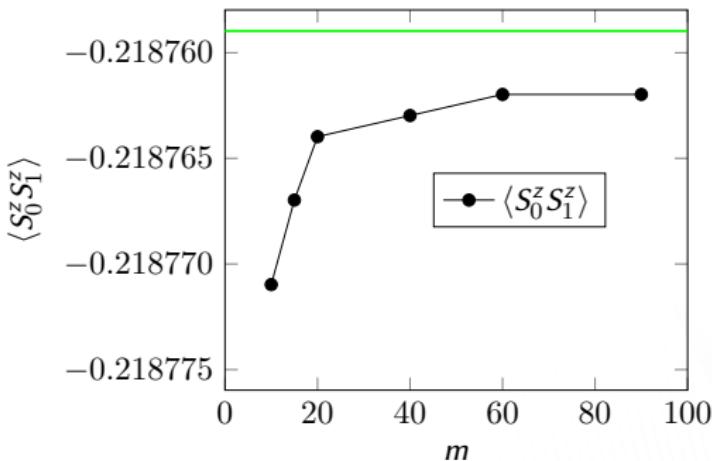
Therefore,  $W^\dagger W = I$  but  $WW^\dagger \neq I$ .

A proper rectangular matrix (rows  $\neq$  cols) has at most one inverse.

# Truncation

## Answer of exercise 12

By modifying the kept states  $m$  in tutorial2016n1, plot  $\langle S_0^z S_1^z \rangle$  vs.  $m$ .



DMRG is systematically correct  
DMRG without truncation is exact.

## **Exercise 14      Pure State Again**

Discuss the DMRG truncation for the pure state of Exercise 2.

## **Exercise 15      Maximally Entangled State Again**

Discuss the DMRG truncation for the maximally entangled state of Exercise 3.

## Exercises

### Exercise 16

Explore the decay of correlations with distance for a 12-site Heisenberg chain.

### Exercise 17

Explore the decay of correlations with distance for a 32-site Heisenberg.

*Hint:* Create input `tutorial2016n2.inp` for 32 sites based on the input `tutorial2016n1.inp` for 12 sites.

### Exercise 18

Given your correlations results, is there short range order in the Heisenberg model on a chain? Is there long range order in the Heisenberg model on a chain? What theorem does your result confirm?

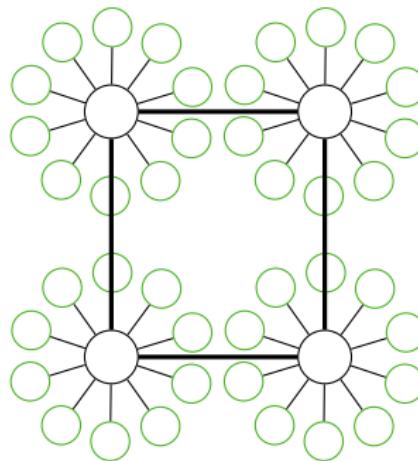
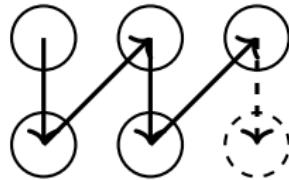
# Ground State DMRG

- 1 DMRG Basics
- 2 Ground State DMRG
- 3 Time, Temperature, Dynamics
- 4 Beyond DMRG

# Models and Geometries

- 1 DMRG Basics
- 2 **Ground State DMRG**
  - 11:00–12:00 Models and Geometries
  - 12:00–01:15 Lunch Break
  - 01:15–02:30 Exercises
- 3 Time, Temperature, Dynamics
- 4 Beyond DMRG

# Geometries

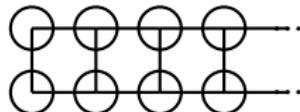


May use area law to estimate complexity

Complexity is exponential of number of links broken when cutting lattice in half.

# Heisenberg 2-leg Ladder

$$H = \sum_{i,j} J_{i,j} \vec{S}_i \cdot \vec{S}_j$$



```
./dmrg -f tutorial2016n20.inp
```

```
./lanczos -f tutorial2016n20.inp
```

```
./dmrg -f tutorial2016n21.inp
```

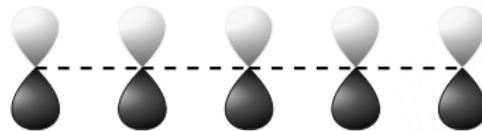
## Hubbard model

$$H = \sum_{i,j,\sigma} t_{i,j} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

```
./dmrg -f tutorial2016n10.inp  
grep lowest runFortutorial2016n10.cout  
./lanczos -f tutorial2016n10.inp
```

```
./dmrg -f tutorial2016n11.inp  
grep lowest runFortutorial2016n11.cout
```

Models can also include multiple orbitals



# Lunch Break

## 1 DMRG Basics

## 2 Ground State DMRG

- 11:00–12:00 Models and Geometries
- **12:00–01:15 Lunch Break**
- 01:15–02:30 Exercises

## 3 Time, Temperature, Dynamics

## 4 Beyond DMRG

## Exercises

### Exercise 19

Confirm that results for a  $2 \times 2$  Heisenberg ladder coincide with those for a 4-site Heisenberg chain with periodic boundary conditions. Create `tutorial2016n3.inp` from `tutorial2016n0.inp` with `IsPeriodicX=1`. Note that this line will be honored only by Lanczos++ and not by DMRG++.

### Exercise 20

Plot the RDM eigenvalues for a  $6 \times 2$  Heisenberg ladder. Compare their decay with that of the 12 site Heisenberg chain.

### Exercise 21

Plot the eigenvalues of a RDM for Hubbard model chain of 6 sites.

## Exercises (continued)

### Exercise 22

Using DMRG, calculate  $\langle \vec{S}_i \cdot \vec{S}_{i+1} \rangle$  for a long (60-site) Heisenberg chain.

*Hint:* ./dmrg -f tutorial2016n40.inp, and then

```
./observe -f tutorial2016n40.inp ss &> sisj.txt
```

### Exercise 23 Back to the 90s

Using DMRG, calculate  $\langle \vec{S}_i \cdot \vec{S}_{i+1} \rangle$  for a long (60-site) Heisenberg chain with two connections  $J$  different. *Hint:* Proceed as before but now using tutorial2016n41.inp. Compare your results for this and the previous exercise to <https://journals.aps.org/prb/abstract/10.1103/PhysRevB.48.10345>

# Exercises (continued)

## Exercise 24

What is the largest size  $L$  that Lanczos alone can simulate in the case of the Hubbard model? *Hint:* Use the result of Exercise 13 and recall that the Hubbard model one-site basis has 4 states instead of 2.

## Exercise 25

How well does DMRG do for a system of “free” electrons? *Hint:* For DMRG, use input tutorial2016n50, which contains the Hubbard model at  $U = 0$ . For the exact calculation you may use FreeFermions.

# FreeFermions

```
cd ../../FreeFermions/examples
perl make.pl
make cicj
./cicj -f tutorial2016n50.inp &> out.txt
grep Energy out.txt
```

## Exercises (continued)

### Exercise 26

For a Hubbard chain of 32 sites, obtain the energy  $E$  vs. density  $n$  at  $U = 8$ .

*Hint:* Use input tutorial2016n60 to obtain the energy for  $n = 0.5$ . Edit the input file, change the density, and rerun to obtain the energy for this other density. Repeat.

TargetElectronsUp	TargetElectronsDown	n
16	16	1.0000
15	15	0.9375
...	...	...

### Exercise 27

Compare these energies with the ones obtained with the Bethe ansatz in the thermodynamic limit. How well does DMRG do? Is a chain of 32 sites a good proxy for the thermodynamic limit? *Hint:* For the Bethe ansatz use Fig. 2 of [Shiba, 1972].

## Exercises (continued)

### Exercise 28      $U \rightarrow \infty$ Hubbard equivalent to Heisenberg

How well is a  $U = 10$  Hubbard model approximated by a Heisenberg model with  $J = 4t^2/U = 0.4t$ ? *Hint:* Obtain energies of each model by using inputs tutorial2016n70 and tutorial2016n71.

### \* Exercise 29      Hubbard model simulated on a 2-leg ladder.

Using DMRG, calculate the energy of a Hubbard model simulated on a 2-leg ladder of size  $8 \times 2$  at half filling for  $U = 0$ . Compare with the exact result. Repeat for the charge correlations  $\langle n_i n_j \rangle$ . *Hint:* Use input tutorial2016n13 with both DMRG++ and FreeFermions. For FreeFermions, use the driver *ninj*.

# Time

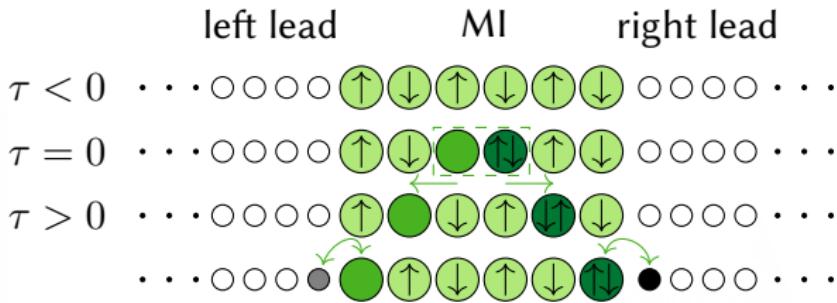


- 1 DMRG Basics
- 2 Ground State DMRG
- 3 Time, Temperature, Dynamics
  - 02:30–03:00 Time
  - 3:00–3:30 Temperature
  - 3:30–4:00 Dynamics
  - 4:00–4:30 Break
- 4 Beyond DMRG

# Motivation: Mott Insulators for Solar Cells



Time propagation of an electronic excitation



For a review see Manousakis, 2010 and references therein

## DMRG Technique: Targeting of States

**Definition:** To *target* a state is to include it in the reduced density matrix.

For example, in

$$\rho_{\alpha,\alpha'}^S = \sum_{\beta} \phi_{\alpha,\beta}^{0*} \phi_{\alpha',\beta}^0 + \sum_{\beta} \phi_{\alpha,\beta}^{1*} \phi_{\alpha',\beta}^1 + \cdots + \sum_{\beta} \phi_{\alpha,\beta}^{n-1*} \phi_{\alpha',\beta}^{n-1}$$

states  $\phi_{\alpha,\beta}^x$ ,  $x = 0, \dots, n - 1$  are targeted.

**Motivation:** States included in the density matrix are then generated with the DMRG algorithm and have similar error profile.

**Example:** For time evolution we need to target at least  $n = 3$  states: the ground state  $|\phi_0\rangle \equiv |gs\rangle$ , the “pulse” state  $|\phi_1\rangle \equiv A_i|gs\rangle$ , and its time evolution  $|\phi_2\rangle \equiv \exp(-iHt)A|gs\rangle$ .

## DMRG Technique: WFT a state



**Definition** The *wave-function transformation* or WFT is the transformation that takes a state in one DMRG basis (one center of orthogonality) into another. White, 1996

**Application** If we want to create a pulse at site  $i$ , then we must apply  $|\phi_1\rangle \equiv A_i|gs\rangle$ , which can only be done when the DMRG center of orthogonality is at  $i$ . We need to “transport” state  $A_i|gs\rangle$  into the next DMRG basis; for that we use the WFT:  $|\phi'_1\rangle = \text{WFT}|\phi_1\rangle$ , *without* reapplying  $A_i$ .

**Application** For ground state calculations,  $\text{WFT}|gs\rangle$  is a good guess for starting the next Hamiltonian diagonalization.

## We use Krylov-space Time Evolution

Tridiagonalize  $H = V^\dagger TV$  starting Lanczos with  $|\phi\rangle$ .  
 $V$  is the matrix of Lanczos vectors and  $T$  is tridiagonal.

$$\exp(\alpha H)|\phi\rangle = \exp(\alpha V^\dagger TV)|\phi\rangle = V^\dagger \exp(-iTt)V|\phi\rangle$$

Diagonalize  $T = S^\dagger DS$ , where  $D$  diagonal.

Finally,\* compute the evolution with

$$\exp(\alpha H)|\phi\rangle_i = \sum_{k,k',k'',j} V_{i,k}^* S_{k,k'}^\dagger \exp(\alpha d_{k'}) S_{k',k''} V_{j,k''} |\phi\rangle_j$$

---

\* This is within a DMRG method, so don't forget to target the appropriate states. For method development, see Schollwöck, 2005 and Manmana et al., 2005. For an implementation, see Alvarez et al., 2011.

## Time Evolution: Exercises

### Exercise 30

### Exciton dynamics in a non-interacting model

$$H = -t \sum_{i=0}^{L-2} (c_i^\dagger c_{i+1} + \text{h.c.})$$

Part(1): Using the definition  $|\psi_i\rangle \equiv c_i^\dagger |0\rangle$ , where  $|0\rangle$  is the vacuum state, verify that the Schröedinger equation

$$H|\Psi\rangle = E|\Psi\rangle$$

is equivalent to the system of equations for the complex coefficients  $\psi_i$ , where  $\langle\psi_i|\Psi\rangle = \langle 0|c_i|\Psi\rangle \equiv \psi_i$

$$-t(\psi_{i-1} + \psi_{i+1}) = E\psi_i \quad i = 0,..L-1. \quad (5)$$

$$\psi_{-1} = \psi_L = 0. \quad (6)$$

*Hint:* Using the *bra*  $\langle\psi_i|$ , evaluate  $\langle\psi_i|H|\Psi\rangle = \langle\psi_i|E|\Psi\rangle$ .

## Time Evolution: Exercises

Part(2): Substitute the *Ansatz*

$$\tilde{\psi}_k = \left( A e^{ikj} + B e^{-ikj} \right) \psi_j$$

in equations (5) and verify that the Hamiltonian eigenvalues are

$$\epsilon_{k_n} = -2t \cos(k_n)$$

while the eigenvectors are

$$\tilde{\psi}_{k_n} \equiv \langle 0 | c_{k_n} | \Psi \rangle = \sqrt{\frac{2}{L+1}} \sum_{i=0}^{L-1} \sin(k_n(i+1)) \psi_i \quad (7)$$

where  $k_n = \frac{n\pi}{L+1}$  with  $n = 1, \dots, L$  are the only possible values verifying the boundary conditions in eq. (6).

## Time Evolution: Exercises

Part(3): Consider a chain with  $L = 6$  sites and  $N = 4$  electrons. Being the model non interacting, the ground state wavefunction and energy are

$$|\Psi\rangle = \prod_{n=1}^N c_{k_n}^\dagger |0\rangle \quad E = \sum_{n=1}^N \epsilon_{k_n}.$$

One can calculate the local densities  $\langle\Psi|n_j|\Psi\rangle$  analytically

$$\langle\Psi|n_j|\Psi\rangle = \frac{2}{L+1} \sum_{n=1}^N \sin^2(k_n(j+1))$$

*Remember:*  $0 \leq j \leq L-1 = 5$ .

Verify with DMRG that you get the correct analytical results

```
./dmrg -f tutorial2016n100.inp  
./observe -f tutorial2016n100.inp '<gs|n?0|gs>'
```

## Time Evolution: Exercises

Part (4): An *exciton* at site  $i$  is given by the wave function

$$|\lambda_i\rangle \equiv c_i^\dagger |\Psi\rangle$$

4.1: Verify that  $|\lambda_i\rangle$  is not an eigenstate of the Hamiltonian  $H$ .

*Hint:* Use that  $H = \sum_{i=1}^L c_{k_i}^\dagger c_{k_i}$ , the *inverse* of eq. (7), and the property  $(c_k)^2 = (c_k^\dagger)^2 = 0$ .

4.2: Verify that the exciton state is not normalized to 1

$$\langle \lambda_i | \lambda_i \rangle = 1 - \frac{2}{L+1} \left( \sum_{n=1}^N \sin^2(k_n(i+1)) \right) < 1 \quad (8)$$

The time-evolution of the exciton state is

$$|\lambda_i(t)\rangle \equiv e^{-iHt} |\lambda_i\rangle$$

## Time Evolution: Exercises

For a chain of  $L=6$  sites and  $N=4$  electrons the local densities as a function of time are given by

$$\begin{aligned} \langle \lambda_i(t) | n_j | \lambda_i(t) \rangle = & \frac{2}{L+1} \sin^2(k_5(i+1)) \left( 1 - \frac{2}{L+1} \sin^2(k_6(j+1)) \right) + \\ & + \frac{2}{L+1} \sin^2(k_6(i+1)) \left( 1 - \frac{2}{L+1} \sin^2(k_5(j+1)) \right) + \\ & + 2 \left( \frac{2}{L+1} \right)^2 \sin(k_5(i+1)) \sin(k_5(j+1)) \sin(k_6(i+1)) \sin(k_6(j+1)) \cos[(\epsilon_{k_5} - \epsilon_{k_6})t] \end{aligned} \quad (9)$$

4.3:

Write<sup>3</sup> to a file the results for  $\langle \lambda_i(t) | n_j | \lambda_i(t) \rangle / \langle \lambda_i | \lambda_i \rangle$  with

```
perl dens.pl [site(i)] [site(j)] [tau] [TotSteps]
> result1.txt
```

*Example:* Use `site(i)=2` and `site(j)=3`, `tau=0.1` and `TotSteps=1000`.

---

<sup>3</sup>The ratio between formulas (8) and (9) are coded in the script `dens.pl`.

## Time Evolution: Exercises

4.4: Obtain the same results with DMRG:

```
./dmrg -f tutorial2016n101.inp
```

Create the datafile `result.txt` for the density (2nd column) at site  $j$  vs. time (1st column)

```
cp ../../dmrgpp/scripts/timeEvolution*.pl .
perl timeEvolution1.pl '<P0|nup|P0>'
0 <runFortutorial2016n101.cout |
perl timeEvolution2.pl 1 [tau] [site(j)] > result.txt
```

*Example:* Use `site(j)=3, tau=0.1`

## Time Evolution: Exercises

Notice that in the file `tutorial2016n101.inp`, we have  
`SolverOptions=TimeStepTargetting, advanceOnlyAtBorder`  
The operator  $c_i^\dagger$  (DMRG++ does the  $\dagger$  operation internally) to create the exciton is included explicitly as

```
TSPOperator=raw
RAW_MATRIX
4 4
0 0 1 0
0 0 0 1
0 0 0 0
0 0 0 0
FERMIONSIGN=1
JMVALUES 0 0
AngularFactor=1
```

The site where the exciton is created is indicated using the flag

`TSPSSite 1 i.`

The other mandatory flag

`TSPLoops 1 6`

means that we are waiting DMRG++ to calculate the ground state first with 6 finite-system sweeps.

## Time Evolution: Exercises

4.5: Obtain the same results with Exact Diagonalization:

```
cp ../FreeFermions/examples/EasyExciton .
./EasyExciton -f tutorial2016n101.inp -p [site(j)]
-i [tau] -t [TotSteps] &> result2.txt
```

*Example:* Use `site(j)=3`, `tau=0.1` and `TotSteps=200`.

*Remember:* `result2.txt` should be cleaned up before plotting!

*Suggestion:* Use `| sed -e 's/(//'` | `sed -e 's/,.*//'` before redirecting to `result2.txt`

4.6 Plot all together (Analytical, DMRG and ED) with any software

```
plot 'result.txt' u 1:2, 'result1.txt' u 1:2,
'result2.txt' u 1:2
```

# Time Evolution: Exercises

## Exercise 31 Green's function in a non-interacting model

For the same Hamiltonian of the previous exercise, the Green's function is defined by ( $\tau > 0$ )

$$G_{j,l}(\tau) \equiv -i\langle\Psi|c_j e^{-i(H-E)\tau} c_l^\dagger|\Psi\rangle.$$

Part(1): Using what you learned in the previous exercise, prove that, for  $L = 6$  and  $N = 4$ , the Green's function is given analytically by<sup>4</sup>

$$iG_{j,l}(\tau) = \left(\frac{2}{L+1}\right) [\sin(k_5(j+1)) \sin(k_5(l+1)) e^{-i\epsilon_{k_5}\tau} + \sin(k_6(j+1)) \sin(k_6(l+1)) e^{-i\epsilon_{k_6}\tau}] \quad (10)$$

*Remember:*  $0 \leq j, l \leq L-1 = 5$ .

---

<sup>4</sup>The formula eq. (10) is coded in the script GreeJltime.pl.

## Time Evolution: Exercises

1.1: Plot the real (2nd column) and imaginary (3rd column) part of the Green's function  $iG_{2,2}(\tau)$  as a function of  $\tau$  (1st column):

```
perl Greenj1time.pl [site(1)] [site(j)] [dtau] [TotSteps]  
> Green.exact.txt
```

*Example:* Use  $\tau=0.1$  and  $\text{TotSteps}=1000$ .

1.2: Obtain the same results with DMRG

```
./dmrg -f tutorial2016n102.inp ':c.txt'
```

where the file `c.txt` is produced with

```
./operator -f tutorial2016n102.inp -l c > c.txt
```

and contains the destruction operator `c` to be measured at all sites  $j$ .

## Time Evolution: Exercises

Create the datafile "Green.dmrg.txt" with the real (2nd column) and imaginary (3rd column) part of the Green's function  $iG_{2,2}(\tau)$  as a function of  $\tau$  (1st column)

```
perl timeEvolution1.pl '<PSI| :c.txt |P0>' 0
< runFortutorial2016n102.cout |
perl timeEvolution2.pl 0 [tau] [site(j)]
> Green.dmrg.txt
```

1.3 Plot all together (Analytical and DMRG) with any software

```
plot 'Green.exact.txt' u 1:2, 'Green.dmrg.txt' u 1:2
plot 'Green.exact.txt' u 1:3, 'Green.dmrg.txt' u 1:3
```

## Time Evolution: Exercises

### Exercise 32      Dynamical spin structure factor

From what you learned in the previous exercises, prepare an input to calculate the quantity

$$S_{j,5}(\tau) = \langle \Psi | S_j^z e^{-i(H-E)\tau} S_5^z | \Psi \rangle.$$

for a Heisenberg model on a chain with  $L = 12$  sites. Run DMRG++ to obtain  $S_{5,5}(\tau)$  as a function of time.

*Hint:* Prepare the operator  $S^z$  in a `sz.txt` file running

```
./operator -f tutorial2016n120.inp -l z > sz.txt
```



# Temperature

## 1 DMRG Basics

## 2 Ground State DMRG

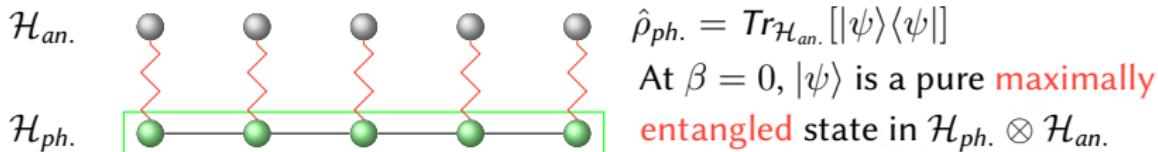
## 3 Time, Temperature, Dynamics

- 02:30–03:00 Time
- **3:00–3:30 Temperature**
- 3:30–4:00 Dynamics
- 4:00–4:30 Break

## 4 Beyond DMRG

## Ancilla DMRG

- **Problem:** DMRG is the ideal method for 1-D systems at  $T = 0$ .  
At  $T > 0$  one needs to know all the eigenstates  $|E_n\rangle$  of the Hamiltonian  $\hat{H}$ ,  $\hat{\rho} = \sum_n \exp(-\beta E_n) |E_n\rangle\langle E_n|$
- **Solution:** Purification of the density operator introducing “ancillas”  
 Verstraete et al., 2004, Zwolak and Vidal, 2004, Feiguin and White, 2005,  
Takahashi and Umezawa, 1975



- METTS approach in  White, 2009; Purification vs. METTS in  
 Binder and Barthel, 2015
- Our work in  Alvarez, 2013 and  Nocera and Alvarez, 2015

# Ancilla DMRG

Example: Heisenberg model on a chain

$$\hat{H} = J \sum_i \hat{S}_i \cdot \hat{S}_{i+1}$$

- Start from the purification  $|\psi_0\rangle$  of the  $\beta = 0$  density operator  $\hat{\rho}_0$

$$|\psi_0\rangle = \bigotimes_{i=0}^{L-1} \left[ \sum_{\sigma=\uparrow,\downarrow} |\sigma\rangle_{ph.} \otimes |\bar{\sigma}\rangle_{an.} \right] \text{ with } \bar{\sigma} = -\sigma, \hat{\rho}_0 = Tr_{\mathcal{H}_A}[|\psi_0\rangle\langle\psi_0|]$$

- Finite temperatures  $\beta > 0$  are reached with imaginary-time evolution with  $\hat{H} = \hat{H}_{ph.} \otimes \mathbf{1}_{an.}$  acting on phys. Hilbert space only

$$|\psi_\beta\rangle = e^{-\frac{\beta}{2}\hat{H}}|\psi_0\rangle \text{ with } \hat{\rho}_\beta \equiv e^{-\beta\hat{H}} = Tr_{\mathcal{H}_A}[|\psi_\beta\rangle\langle\psi_\beta|]$$

- Observables:  $\langle \hat{O} \rangle_\beta \equiv \frac{Tr(\hat{\rho}_\beta \hat{O})}{Tr(\hat{\rho}_\beta)} = \frac{\langle \psi_\beta | \hat{O} | \psi_\beta \rangle}{\langle \psi_\beta | \psi_\beta \rangle} = \frac{\sum_n \exp(-\beta E_n) \langle E_n | \hat{O} | E_n \rangle}{\sum_n \exp(-\beta E_n)}$

# Ancilla DMRG

Heisenberg model: “Grand-Canonical” Purified state

$$|\psi_0\rangle = \bigotimes_{i=0}^{L-1} \left[ \sum_{\sigma=\uparrow,\downarrow} |\sigma\rangle_{ph.} \otimes |\bar{\sigma}\rangle_{an.} \right]$$

How do we get a Grand-Canonical purified state “workable” for DMRG?  
We need an “Entangler” Hamiltonian!

$$\hat{H}_{Entangler}^{GC} = - \sum_i S_i^+ \otimes S_{a(i)}^- + \text{h.c.}$$

One has  $\hat{H}_{Entangler}^{GC} |\psi_0\rangle = E^{GC} |\psi_0\rangle \rightarrow$  only ground state DMRG needed!

$\hat{H}^{GC}$  is “local” on the rungs  $\rightarrow$  DMRG is very fast!

## Temperature: Exercises

### Exercise 33 Single 1/2 spin at finite temperature

Hilbert space Basis:  $|\downarrow\rangle, |\uparrow\rangle$

$$\hat{H} = h\hat{S}^z \rightarrow \begin{pmatrix} -h/2 & 0 \\ 0 & h/2 \end{pmatrix} \quad h > 0$$

$$E_{GS} = -h/2 \quad |\Psi_{GS}\rangle = |\downarrow\rangle \rightarrow \hat{\rho}_{GS} \equiv |\Psi_{GS}\rangle\langle\Psi_{GS}| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\text{Thermal Density Matrix: } \hat{\rho}_{th} \equiv \frac{e^{-\beta\hat{H}}}{Z} \rightarrow \begin{pmatrix} e^{\beta h/2}/Z & 0 \\ 0 & e^{-\beta h/2}/Z \end{pmatrix}$$

$$\text{Partition Function: } Z \equiv \text{Tr} \left( e^{-\beta\hat{H}} \right) = e^{\beta h/2} + e^{-\beta h/2}$$

## Temperature: Exercises

Verify that

$$1) T = 0 \rightarrow \hat{\rho}_{th} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad T \rightarrow \infty \rightarrow \hat{\rho}_{th} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

$$2) \langle E \rangle_\beta \equiv \frac{\text{Tr}(\hat{H}\hat{\rho}_{th})}{Z} = -h/2 \tanh(\beta h) \quad \left\{ \begin{array}{ll} T = 0 & \langle E \rangle_\beta = -h/2 \\ T \rightarrow \infty & \langle E \rangle_\beta = 0 \end{array} \right.$$

### Exercise 34 Single 1/2 spin with Ancilla

Hilbert space  $\mathcal{H}_r \otimes \mathcal{H}_a$ ; Basis:  $|\downarrow_r, \uparrow_a\rangle, |\downarrow_r, \downarrow_a\rangle, |\uparrow_r, \uparrow_a\rangle, |\uparrow_r, \downarrow_a\rangle$

(1) Verify that

$$\hat{H}_r \otimes \mathbf{1}_a = h\hat{S}_r^z \otimes \mathbf{1}_a \rightarrow \begin{pmatrix} -h/2 & 0 & 0 & 0 \\ 0 & -h/2 & 0 & 0 \\ 0 & 0 & h/2 & 0 \\ 0 & 0 & 0 & h/2 \end{pmatrix}$$

## Temperature: Exercises

(2) Given the state  $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\downarrow_r, \uparrow_a\rangle - |\uparrow_r, \downarrow_a\rangle)$

Calculate the reduced density matrix of the real site ( $2 \times 2$  matrix!):

$\hat{\rho}_r \equiv \text{Tr}_a(|\Psi\rangle\langle\Psi|)$ . How does it look like?

(3) Verify that  $|\Psi(\beta)\rangle = e^{-\frac{\beta}{2}\hat{H}}|\Psi\rangle = \frac{1}{\sqrt{2}}(e^{\beta h/4}|\downarrow_r, \uparrow_a\rangle - e^{-\beta h/4}|\uparrow_r, \downarrow_a\rangle)$

*Hint:* When a matrix  $M$  is diagonal, its exponential  $e^M$  is equal to a matrix with diagonal elements equal to the exponential of the diagonal elements of  $M$ !

(4) Calculate the reduced density matrix of the real site ( $2 \times 2$  matrix!):

$\hat{\rho}_r(\beta) \equiv \text{Tr}_a(|\Psi(\beta)\rangle\langle\Psi(\beta)|)$ . How does it look like?

(5) Calculate  $\langle\Psi(\beta)|\Psi(\beta)\rangle$ , how does it compare with the partition function  $Z$  of the previous exercise?

(6) Calculate  $\frac{\langle\Psi(\beta)|\hat{H}|\Psi(\beta)\rangle}{\langle\Psi(\beta)|\Psi(\beta)\rangle}$ . How does it compare with  $\langle E \rangle_\beta$  calculated in the previous exercise?

## Temperature: Exercises

### Exercise 35 Single 1/2 spin Entangler Hamiltonian

Verify that the *state*  $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\downarrow_r, \uparrow_a\rangle - |\uparrow_r, \downarrow_a\rangle)$  is the ground state of the Hamiltonian

$$\hat{H}_E = - (S_r^+ \otimes S_a^- + S_a^+ \otimes S_r^-)$$

*Hint:*

$$\hat{H}_E = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

## Temperature: Exercises

### Exercise 36 Heisenberg chain at finite temperature

Calculate the energy of a Heisenberg chain with  $L = 6$  sites and  $J = -1$  with DMRG

- Find the ground state of the Entangler Hamiltonian.  
`./dmrg -f tutorial2016n1800.inp`
- Evolve in imaginary time with the real Hamiltonian.  
`./dmrg -f tutorial2016n1801.inp`

In the input file, the line

`SolverOptions=twositedmrg, restart, TargetingAncilla`

means that we are *restarting* from the ground state and evolving in imaginary time.

## Temperature: Exercises

Verify that at large  $\beta$  you get the ground state energy.

- Run the `getEnergyAncilla.pl` script and get the energy  $\langle \hat{H} \rangle_\beta$  for large  $\beta$

```
perl getEnergyAncilla.pl [betaprime] time
< runFortutorial2016n1801.cout
```

Where `betaprime` is the actual value  $\beta' = \beta = 1/(2T)$ .

*Example:* Use `betaprime=10`.

- Obtain the ground state energy of `tutorial2016n1802.inp`

Verify you get the same results of fig.1 of Ref.  Nocera and Alvarez, 2015.



# Dynamics

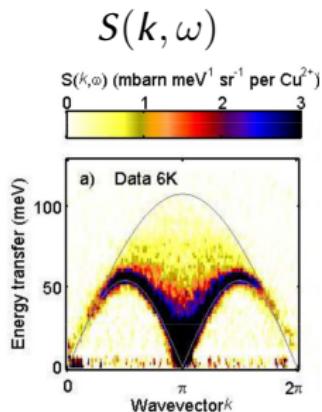
## Real Frequency Properties

- 1 DMRG Basics
- 2 Ground State DMRG
- 3 Time, Temperature, Dynamics
  - 02:30–03:00 Time
  - 3:00–3:30 Temperature
  - 3:30–4:00 Dynamics
  - 4:00–4:30 Break
- 4 Beyond DMRG

# Dynamical response functions: Experiments reveal complex quantum phenomena

1D Heisenberg  $\text{KCuF}_3$

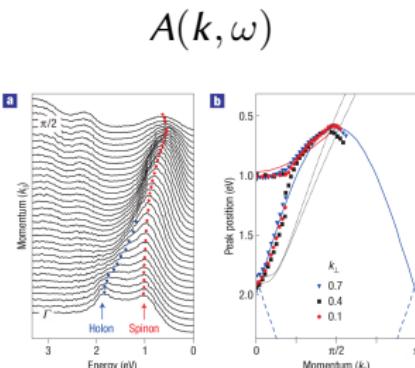
Lake et al., 2013



Spinon excitations

1D Mott Insulator  $\text{SrCuO}_2$

Kim et al., 2006



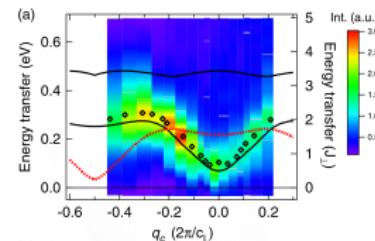
Spin-charge separation

Two-leg ladder

$\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$

Schlappa et al., 2009

$I(k, \omega)$



Triplon excitations  
of a spin liquid

# Compute $S(q, \omega)$ , $A(q, \omega)$ with DMRG

## Methods

- Evolve in time, then Fourier transform into  $\omega$   
[White and Affleck, 2008]
- Continued fraction approach [Hallberg, 1995]

$$S(q, \omega) = \langle gs | S_q^- \frac{1}{\omega + i\delta - (H - E_0)} S_q^+ | gs \rangle$$

- Correction vectors [Kühner and White, 1999, Pati et al., 1999, Kühner et al., 2000.]
- Other methods. Active area of research  
[Jeckelmann, 2002, Dargel et al., 2011, Dargel et al., 2012.]
- Our work: [Nocera and Alvarez, 2016]

## Correction Vector DMRG

We are interested in the calculation of the Green's function

$$G(z) = -\frac{1}{\pi} \langle \psi_0 | \hat{B} \frac{1}{z + E_0 - \hat{H}} \hat{A} | \psi_0 \rangle,$$

- $|\psi_0\rangle$  is the ground state of some Hamiltonian  $\hat{H}$  with ground-state energy  $E_0$ ,
- $\hat{A}$  and  $\hat{B}$  are operators associated with the dynamical correlation function to be calculated (ex.  $S^+$ ,  $S^z$ ,  $S^-$ ,  $c^\dagger$ ,  $c$ ),
- $z \equiv \omega + i\eta$ , where  $\omega$  is the real frequency and  $\eta$  is a positive constant (giving broadening of the peaks).

## Correction Vector DMRG

The *correction-vector* is defined by

$$|x(z)\rangle = \frac{1}{z + E_0 - \hat{H}} |A\rangle, \text{ where } |A\rangle \equiv \hat{A}|\psi_0\rangle \text{ is assumed real.}$$

Assuming  $|x(z)\rangle$  is *known*, how to compute  $G(z)$  with DMRG?

Answer: Use multi-target approach.

- At each step of the DMRG algorithm, target the ground state of the system  $|\psi_0\rangle$ , the vector  $|A\rangle$  and the  $|x(z)\rangle$  in the reduced density matrix, for each frequency value  $\omega$  and broadening  $\eta$ .
- Calculate  $G(z)$  using

$$G(z) = -\frac{1}{\pi} \langle \psi_0 | \hat{B} | x(z) \rangle.$$

## Correction Vector DMRG

How do we compute the correction-vector?..Active area of research!

Most used method is Conjugate-Gradient. Kühner and White, 1999

We use a Krylov-space method, recently proposed by us in  
ref. Nocera and Alvarez, 2016.

The correction-vector  $|x(z)\rangle$  is calculated *directly* as

$$|x(z)\rangle = V^\dagger S^\dagger \frac{1}{E_0 + \omega - D + i\eta} SV|A\rangle,$$

- $D$  is the diagonal form of the Hamiltonian operator  $\hat{H}$
- We assume that  $\hat{H}|A\rangle \simeq V^\dagger TV|A\rangle = V^\dagger S^\dagger DSV|A\rangle$
- $V$  is the matrix of the Lanczos vectors spanning the Krylov space
- $T$  is the representation of the Hamiltonian in tridiagonal form

## Dynamics: Exercises

### Exercise 37 LDOS of a non-interacting chain

- From Ex. 31, take formula (10) and Fourier Transform it.

*Hint:* Remember you need to add a imaginary time constant such that the following integral is convergent

$$\int_0^{+\infty} d\tau (-i) e^{i(\omega - \epsilon_k + i\eta)\tau} = \frac{1}{\omega - \epsilon_k + i\eta}$$

- Verify that

$$G_{j,l}(\omega) = \left( \frac{2}{L+1} \right) \left[ \frac{\sin(k_5 j) \sin(k_5 l)}{\omega - \epsilon_{k_5} + i\eta} + \frac{\sin(k_6 j) \sin(k_6 l)}{\omega - \epsilon_{k_6} + i\eta} \right] \quad (11)$$

The local density of states at site  $j$  is:  $N_j(\omega) \equiv -\text{Im}[G_{j,j}(\omega)]$

## Dynamics: Exercises

- Fourier Transform the time signal `Green.exact.txt` obtained in 1.1 of Ex. 31.

*Hint:* The script `FourierTransform.pl` helps you in FT a time signal on a finite interval of time.

```
perl FourierTransform.pl L tau file wmax dw w0
```

*Example:* Use `L=6, tau=0.1, file=Green.exact.txt, wmax=3, dw=0.1, w0=0`.

- Compare what you obtained with the exact  $N_j(\omega)$

*Hint:* The script `Njomega.pl` prints the  $N_j(\omega)$

```
perl Njomega.pl [site(j)] [eta] [dw] [ToTw]  
> Njomega.exact.txt
```

*Example:* Use `site(j)=2, eta=0.05, dw=0.1, ToTw=30`.

## Dynamics: Exercises

- Calculate  $N_j(\omega)$  with correction-vector DMRG.

Recall that:

$$N_j(\omega) = -\text{Im} \langle \psi_0 | c_j \frac{1}{\omega + E_0 - \hat{H} + i\eta} c_j^\dagger | \psi_0 \rangle,$$

The input `tutorial2016n140.inp` is provided.

Notice the flag:

`SolverOptions=CorrectionVectorTargetting`

which means we are *targetting* the correction-vector.

- Choose appropriately dw, w0 and ToTw

```
#OmegaBegin=0  
#OmegaStep=0.1  
#OmegaTotal=30
```

## Dynamics: Exercises

- The observable  $c_j$  to measure *in situ* at each site  $j$  is set with the flag `#Observable=c`, which is produced and printed in the file `c.txt` with

```
./operator -f tutorial2016n140.inp -l c > c.txt
```

- The operator  $c_j$  (DMRG++ does the  $\dagger$  operation internally) to be applied at site `TSPSite 1 j` is included explicitly in the input as

```
TSPOperator=raw
RAW_MATRIX
4 4
0 0 1 0
0 0 0 1
0 0 0 0
0 0 0 0
FERMIONSIGN=1
JMVALUES 0 0
AngularFactor=1
```

## Dynamics: Exercises

- Run dmrng for each frequency  $\omega$ .
  - Produce the inputs for each  $\omega$  with the script manyOmegas.pl  
Notice the flag CorrectionVectorOmega=\$omega and the line  
`./dmrg -f $$input ':c.txt' &> out$$ind.txt`  
in the file tutorial2016n140.pbs.
  - Run

```
perl manyOmegas.pl tutorial2016n140.inp
tutorial2016n140.pbs test
```
  - Verify you produced the inputs `input$omega.inp`, where `$omega` is the current frequency step to be processed.
- Process the results with the script procOmegas.pl

```
perl procOmegas.pl -f tutorial2016n140.inp
-S sitej &> Njomega.dmrng.txt
```
- Compare the results with those you obtained in above and printed in `Njomega.exact.txt`

# Break

- 1 DMRG Basics
- 2 Ground State DMRG
- 3 Time, Temperature, Dynamics
  - 02:30–03:00 Time
  - 3:00–3:30 Temperature
  - 3:30–4:00 Dynamics
  - 4:00–4:30 Break
- 4 Beyond DMRG

# Beyond DMRG

## Current Research in DMRG Related Methods

- 1 DMRG Basics
- 2 Ground State DMRG
- 3 Time, Temperature, Dynamics
- 4 Beyond DMRG

# Hamiltonian Complexity

- The area law has been rigorously proved by M. Hastings Hastings, 2007
- A DMRG-like algorithm has been rigorously proved to be in  $P$   
 Aharonov et al., 2010

*“In recent years we have seen the birth of a new field known as Hamiltonian complexity lying at the crossroads between computer science and theoretical physics. Hamiltonian complexity is directly concerned with the question: how hard is it to simulate a physical system?”*

*Tobias J. Osborne in* Osborne, 2012

# Complexity Classes

P is the class of decision problems that can be solved in polynomial computational time by a (deterministic) Turing machine.<sup>5</sup>

NP is the class of decision problems that can be verified in polynomial computational time by a (deterministic) Turing machine.

NP-complete are the hardest<sup>6</sup> problems in NP. The classical Ising model  $H = \sum_{i,j} J_{ij} S_i^z S_j^z$  is NP-complete.

MA is the class of decision problems that can be solved with the help of an all powerful but sometimes deceptive oracle.

QMA is the class of decision problems that can be verified with the help of an all powerful but sometimes deceptive oracle. The local Hamiltonian problem is QMA-complete<sup>7</sup>.

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<sup>5</sup>For rigorous definitions, see, for example, [Arora and Barak, 2009](#).

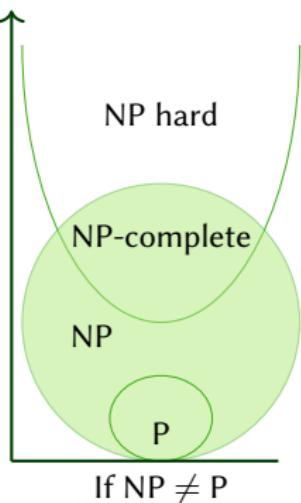
<sup>6</sup>Any other problem reduces to it in polynomial time.

<sup>7</sup>when formulated as a decision problem

# Quantum Hamiltonian Complexity: Not even in NP!



- NP problems are problems where a solution can be verified in polynomial time.
- Given  $\vec{v}$  one **cannot** verify in polynomial time if it's an eigenvector of  $H$ ....Because  $H$  has rank exponential in the number of sites.
- The Hamiltonian problem is in class **Quantum Merlin Arthur\***



\*See Schuch et al., 2008 Schuch and Verstraete, 2009

Cubitt and Montanaro, 2013 Osborne, 2013

Liu et al., 2007 Aharonov and Naveh, 2002

# DMRG in the Matrix Product State language

## Why a different formulation of DMRG?

DMRG in the MPS language enables a better understanding of the algorithm, and its generalizations.

# Matrix Product States

Consider a Heisenberg model on  $N$  even sites. States of the computational basis are of the form  $|\sigma_0\sigma_1 \cdots \sigma_{N-1}\rangle$  where  $\sigma_i \in \{\uparrow, \downarrow\}$  for  $0 \leq i < N$ . Matrix product states are of the form

$$\sum_{\{\sigma\}} \sum_{\{i\}} A_{0,i_1}^0(\sigma_0) A_{i_1,i_2}^1(\sigma_1) A_{i_2,i_3}^2(\sigma_2) \cdots A_{i_{N-1},0}^{N-1}(\sigma_{N-1}) |\sigma_0\sigma_1 \cdots \sigma_{N-1}\rangle$$

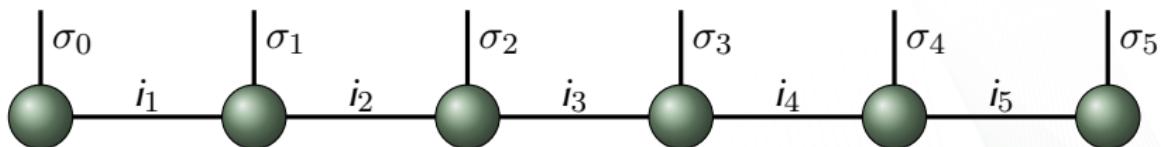
where  $A_0$  is a  $1 \times D$  matrix,  $A_1$  is a  $D \times D^2$  matrix,  $A_{N/2-1}$  is a  $D^{N/2-1} \times D^{N/2}$ ,  $A_{N/2}$  is a  $D^{N/2} \times D^{N/2-1}$ , ...,  $A^{N-2}$  is a  $D^2 \times D$  matrix, and  $A^{N-1}$  is a  $D \times 1$  matrix.

$$\sum_{\{\sigma\}} \sum_{\{i\}} \text{Tr} (A^0(\sigma_0) A^1(\sigma_1) A^2(\sigma_2) \cdots A^{N-1}(\sigma_{N-1})) |\sigma_0\sigma_1 \cdots \sigma_{N-1}\rangle$$

## DMRG in Matrix Product State Language

The DMRG algorithm is equivalent to the optimization<sup>8</sup> of an MPS for the matrices  $A^i(\sigma_i)$  [Rommer and Ostlund, 1997]. In other words, the matrices  $A$  can be truncated efficiently in (non critical) one-dimensional systems.  $A_0$  is a  $1 \times D$  matrix,  $A_1$  is a  $D \times D^2$  matrix,..., until  $A^k$  is a  $D^k \times m$  matrix, where  $D^k < m < D^{k+1}$ .

$$\sum_{\{\sigma\}} \sum_{\{i\}} A_{0,i_1}^0(\sigma_0) A_{i_1,i_2}^1(\sigma_1) A_{i_2,i_3}^2(\sigma_2) \cdots A_{i_{N-1},0}^{N-1}(\sigma_{N-1}) |\sigma_0 \sigma_1 \cdots \sigma_{N-1}\rangle$$



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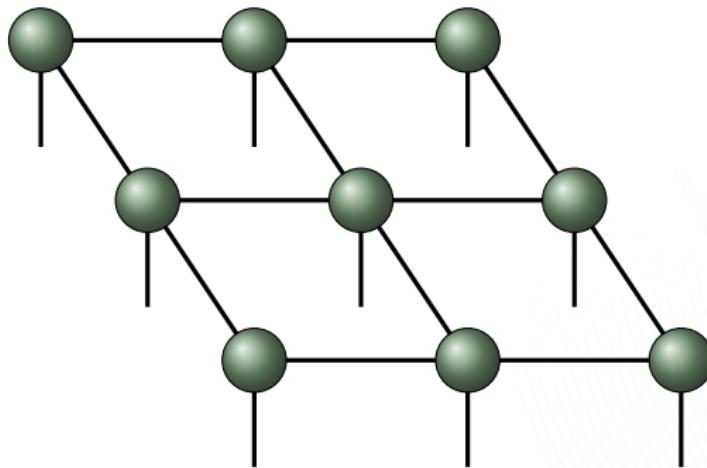
<sup>8</sup>For the optimization procedure see [Schollwöck, 2010]. iTensor is an MPS code by M. Stoudenmire and S. White at <http://itensor.org>

# Tensors: PEPS

MPS

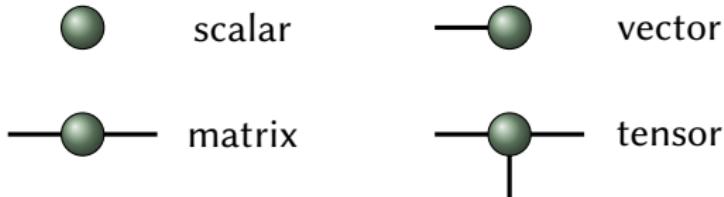


Projected Entangled Pair States or PEPS Verstraete and Cirac, 2004

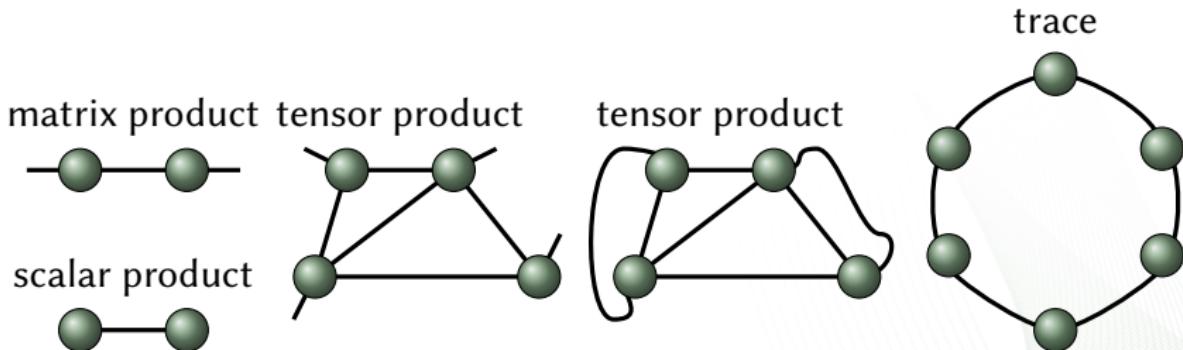


# More Tensors

## Tensor Diagrams



## Tensor Contractions (Adapted from Orus, 2014)



# The Race to Solve the 2D Problem

Because many materials need not just 1D simulation but 2D modeling, finding an efficient representation of the **2D problem** and solving it is a major area of study  Stoudenmire and White, 2011

We've already mentioned PEPS. Another effort has been the multi-scale-renormalization ansatz or **MERA**  Vidal, 2008.

# Tutorial Aims

At the end of this tutorial,

- ① you will have understood the correlated electron problem in condensed matter,
- ② you will have understood the solution to that problem based on the DMRG.
- ③ By following through the worked exercises during the tutorial, you will have a working knowledge of ground state DMRG applied to models of quantum spins, and correlated electrons.
- ④ You will be ready to expand your knowledge of DMRG into time evolution, temperature, and dynamics.
- ⑤ Finally, you will know enough to be able to follow current research in the area of DMRG, and understand the current race to solve the two-dimensional problem.

## After the Tutorial

- Where can I find additional resources? For example, see E. Jeckelmann's webpage at <https://www.itp.uni-hannover.de/~jeckelm/dmrg/>
- Where are these slides? [git pull https://github.com/g1257/dmrg101](https://github.com/g1257/dmrg101)
- Where's the scientific software? At <https://github.com/g1257/>  
Mirror at [https://code.ornl.gov/u/gonzalo\\_3/projects](https://code.ornl.gov/u/gonzalo_3/projects)
- How can I contact you? We have a public mailing list at [dmrgpp@ornl.gov](mailto:dmrgpp@ornl.gov) and messages will appear at <https://elist.ornl.gov/mailman/listinfo/dmrgpp>
- How can I contribute? See next slide

# Please contribute!

## What to contribute

- Comments and Criticisms of this Tutorial
- Solutions to Exercises
- Questions and Answers
- Documentation fixes and additions
- Computer codes, patches, pull requests
- New models and geometries

## Should I write my own computer codes?

Write only a proof of principle to learn methods. For production, collaborate and use computer codes from reputable software projects and groups.

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<sup>8</sup>We are writing the contribution guidelines and will post them soon.

# Thanks!

## Thanks

Thanks to all of you for participating in this workshop. Thanks also to E. F. Dumitrescu, T. S. Humble, J. Jakowski, N. Patel, M. S. Summers for your help.

## Credit Line

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Thanks to  Office of  
Science

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Tikz was used for some figures.