DMRG 101: Introduction to Theory and Practice

When: August 12, 2016

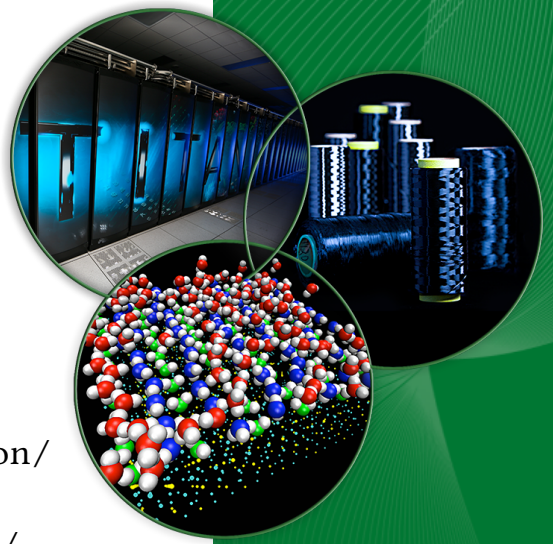
Where: ORNL, Oak Ridge, TN, USA

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



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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.

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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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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
```


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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`

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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`

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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
```


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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
```


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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

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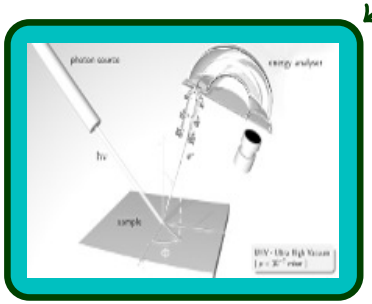
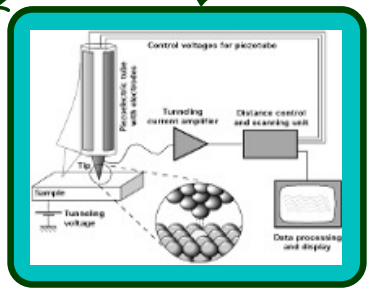
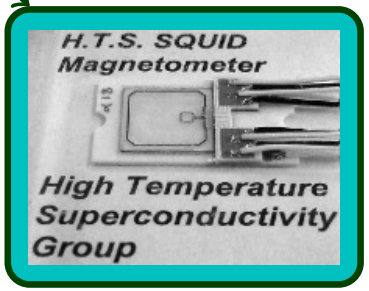
Experiment and Theory

Experiment







$S(k,\omega)$ $A(k,\omega)$ $N(r,\omega)$ Magnetization SC Gaps

Theory

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First Quantization of Condensed Matter

$$H = H_n + H_{1e} + H_{e-e}, \tag{1}$$

where

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

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

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

What's the problem?

The problem is to solve the Schroëdinger 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 easy to study....But not always.

Some materials are 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.*

* See Dagotto, 2005.

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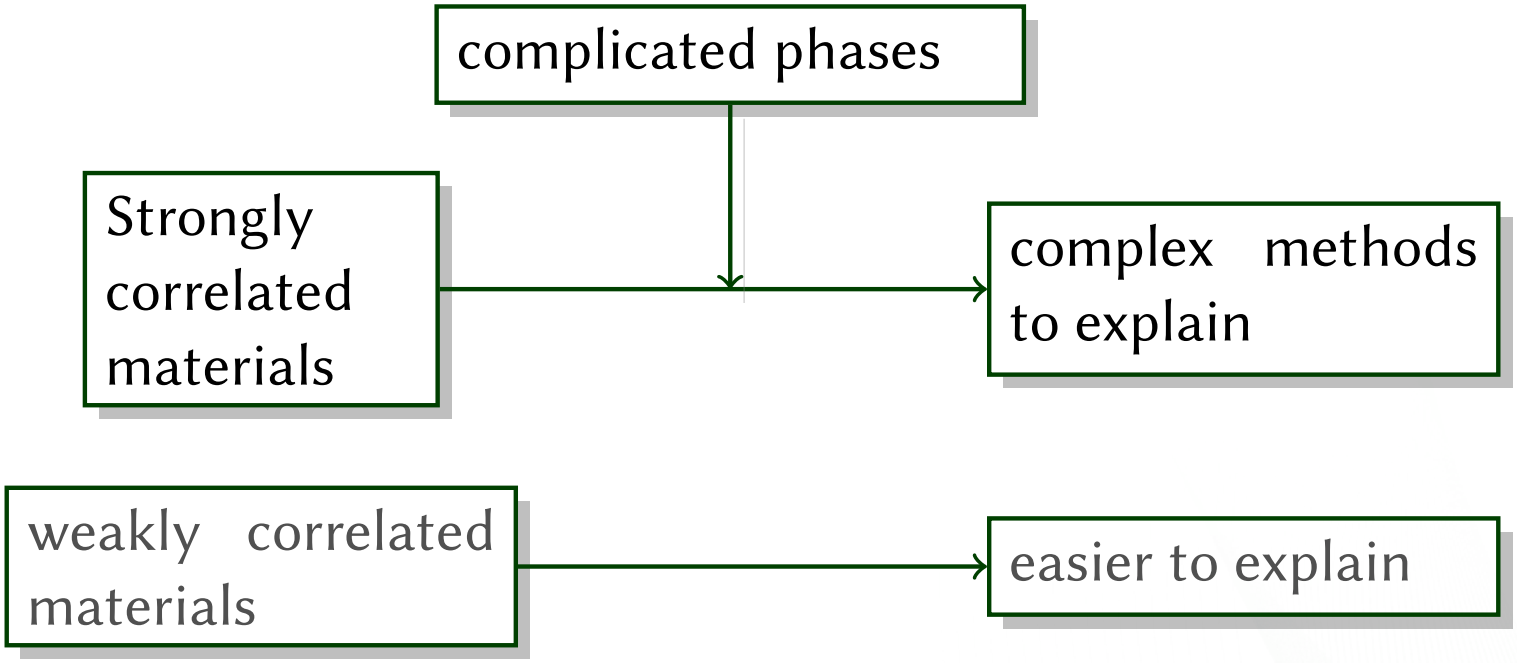
What causes the energetically-close phases?

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?



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Why are these materials costly to study?

Answer: Because the "standard one-electron model" of metals breaks down. LDA cannot be used

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

And accurate approaches are computationally costly.

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Condensed Matter in Second Quantization

The Hilbert Space

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

$$c^\dagger_{i\uparrow}|0>=|\cdots\uparrow\cdots\rangle$$

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[1]

[1] Spalek and Oleś, 1977, Hubbard, 1963, Hubbard, 1964

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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

$\bigcirc \quad \bigcirc \;\Big|\; \uparrow \quad \bigcirc \;\Big|\; \bigcirc \quad \uparrow \;\Big|\; \downarrow \quad \bigcirc \;\Big|\; \cdots$

What are the possible quantum numbers $(N_\uparrow, N_\downarrow)$? See 23.
How many states are there with a given $(N_\uparrow, N_\downarrow)$? $C^N_{N_\uparrow} C^N_{N_\downarrow}$.
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

$$\bigcirc \quad \bigcirc \;\Big|\; \uparrow \quad \bigcirc \;\Big|\; \bigcirc \quad \uparrow \;\Big|\; \downarrow \quad \bigcirc \;\Big|\; \cdots$$

$N_\uparrow$	$N_\downarrow$	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

$$\begin{pmatrix}
\mathrm{X} & & & & & & & & & & & & & & & \\
 & \mathrm{X} & \mathrm{X} & & & & & & & & & & & & & \\
 & \mathrm{X} & \mathrm{X} & & & & & & & & & & & & & \\
 & & & \mathrm{X} & \mathrm{X} & & & & & & & & & & & \\
 & & & \mathrm{X} & \mathrm{X} & & & & & & & & & & & \\
 & & & & & \mathrm{X} & \mathrm{X} & \mathrm{X} & \mathrm{X} & & & & & & & \\
 & & & & & \mathrm{X} & \mathrm{X} & \mathrm{X} & \mathrm{X} & & & & & & & \\
 & & & & & \mathrm{X} & \mathrm{X} & \mathrm{X} & \mathrm{X} & & & & & & & \\
 & & & & & \mathrm{X} & \mathrm{X} & \mathrm{X} & \mathrm{X} & & & & & & & \\
 & & & & & & & & & \mathrm{X} & & & & & & \\
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 & & & & & & & & & & & \mathrm{X} & \mathrm{X} & & & \\
 & & & & & & & & & & & & & \mathrm{X} & \mathrm{X} & \\
 & & & & & & & & & & & & & \mathrm{X} & \mathrm{X} & \\
 & & & & & & & & & & & & & & & \mathrm{X}
\end{pmatrix}$$

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

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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 Schroëdinger 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 $v^T Ov$.

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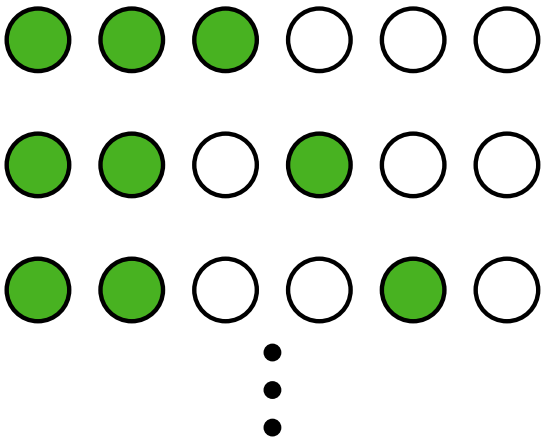
Condensed Matter in Second Quantization

The Problem is Exponential

Example: Heisenberg model, 6 sites, $S^z = 0$: $C_3^6 = 20$ states



For large N we have Stirling's approximation

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

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...
- 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
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The Heisenberg model spin $1/2$

$S_i^\dagger$ 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.

● $m = 1/2$

○ $m = -1/2$

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

Example: 4 sites

○ ○ ○ ○ | ● ○ ○ ○ | ...

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

○ ○ ● ● | ○ ● ○ ● | ...

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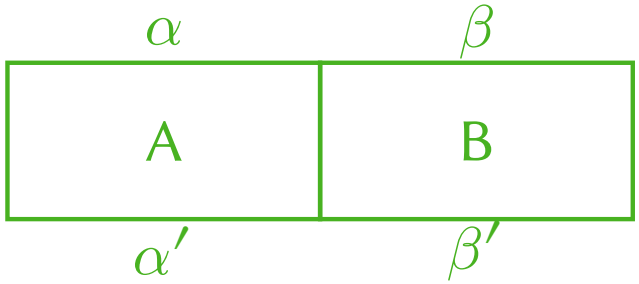
The Reduced Density Matrix



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

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

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

$$\langle\psi|A \otimes I|\psi\rangle = \sum_{\alpha,\alpha',\beta} \psi^*_{\alpha,\beta} A_{\alpha,\alpha'} \psi_{\alpha',\beta} = \sum_{\alpha,\alpha'} A_{\alpha,\alpha'} \sum_{\beta} \psi^*_{\alpha,\beta} \psi_{\alpha',\beta}$$

$$= \sum_{\alpha,\alpha'} A_{\alpha,\alpha'} \rho^S_{\alpha',\alpha} = Tr(A\rho^S) = Tr(AW^\dagger D W) = Tr(WAW^\dagger D) =$$

$$= \sum_{\alpha} \bar{A}_{\alpha,\alpha} d_\alpha = \sum_{\alpha<m} \bar{A}_{\alpha,\alpha} d_\alpha + E(m), \text{where the error } E(m) \text{ is}$$

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

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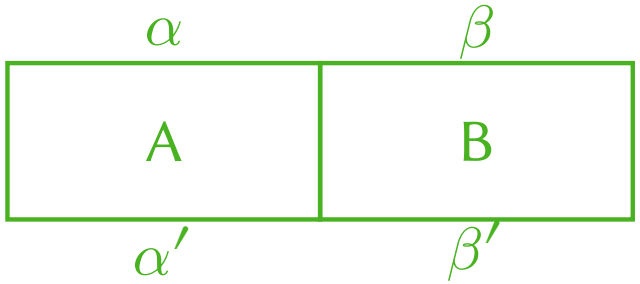
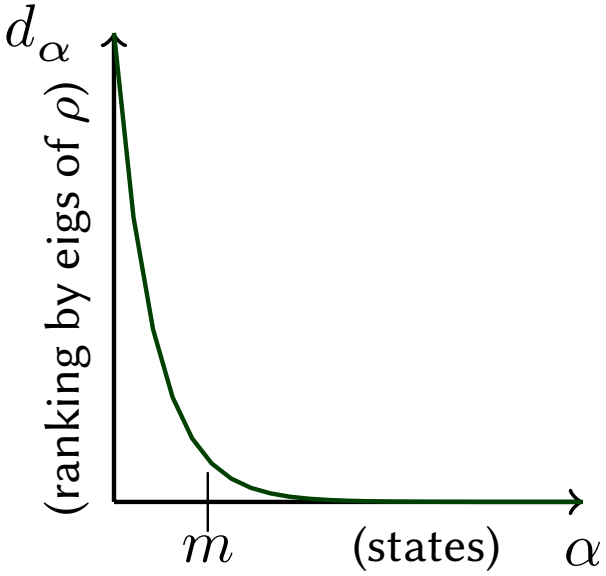
The Eigenvalues of the Density Matrix



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

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



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

$$\rho^A_{\alpha,\alpha'} \equiv \sum_\beta \psi^*_{\alpha,\beta} \psi_{\alpha',\beta}$$

Notation

$A \equiv S \equiv$ left block $\equiv$ "the system"

$B \equiv E \equiv$ right block $\equiv$ "the environ"

$A \cup B \equiv$ "superblock"

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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 λ is an eigenvalue of the reduced density matrix, then $0 \leq \lambda \leq 1$. *Hint:* Use the definition of ρ, and that $\sum_{\alpha,\beta} |\psi_{\alpha,\beta}|^2 = 1$, that is, that ψ is normalized.

Exercise 2 Pure State

If $\psi_{\alpha,\beta} = v_\alpha w_\beta$ for some 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 $n = 3$.

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Downloading the computer codes

Please see slide 6.

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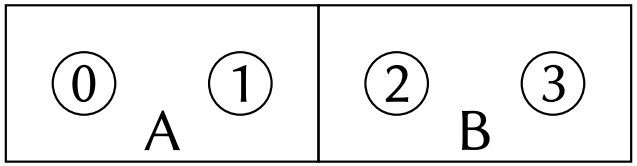
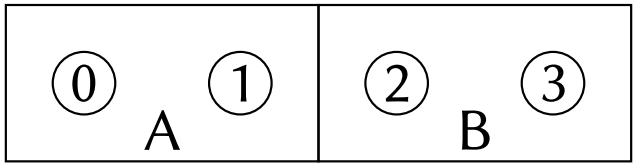
Example: 4-site Heisenberg



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

TotalNumberOfSites=4	
Model=Heisenberg	Model
HeisenbergTwiceS=1	$S = 1/2$ Heisenberg
Connectors 1 1.0	$J_{\pm} = 1.0$, 1 Connector given
GeometryOptions=ConstantValues	Spacially constant connectors
Connectors 1 1.0	$J_z = 1.0$
TargetElectronsTotal=4	FIXME
TargetSzPlusConst=2	# 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
```

[1] All numbers rounded here and elsewhere in these slides.

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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
$A =$	$S_0^z S_1^z$
$2S_0^z =$	$diag(1, 1, -1, -1)$
$2S_1^z =$	$diag(1, -1, 1, -1)$
$4S_0^z S_1^z =$	$diag(1, -1, -1, 1)$

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

-0.25	...	...	...
...	0.25	...	...
...	...	0.25	...
...	...	...	-0.25

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Truncation

Keeping all states we get[2]

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

$d_0 = d_1 = d_2 = 0.022$ 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

$$Error(m = 1) = (-0.25)d_0 + 0.25d_1 + 0.25d_2 = 0.005,$$

[2] Warning: Truncated numbers throughout.

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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 $C^N_{N_\uparrow} C^N_{N_\downarrow}$ 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?

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DMRG Algorithm

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4. Beyond DMRG

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