Diagonalization Solvers for Electronic Collective Phenomena in Nanoscience

Time, Temperature, and Dynamics in the Density Matrix Renormalization Group Algorithm

G. Alvarez

Oak Ridge National Laboratory

CNMS User Meeting
September 19-20, 2011
CNMS, Oak Ridge National Laboratory
Oak Ridge, TN

Outline

Defining the Theory Problem

$$H = -\sum_{i=1}^{Nc} \frac{\hbar^2 \nabla^2}{2m_e} + \frac{e^2}{4\pi\epsilon_0} \sum_{i}^{N_c} \sum_{i<j}^{N+c} \frac{1}{|\vec{r}_i - \vec{r}_j|} + \cdots \quad (1)$$

- Ground state energies, Magnetic and spin orders and correlations. Magnetization measurements: SQUID
- Superconducting orders and gaps. Superconducting gaps: Andreev spectroscopy
- $A(k,\omega)$. ARPES measurements
- $N(r,\omega)$. STM measurements
- $S(k,\omega)$. neutron scattering measurements

Defining the Theory Problem

$$H = -\sum_{i=1}^{Nc} \frac{\hbar^2 \nabla^2}{2m_e} + \frac{e^2}{4\pi\epsilon_0} \sum_{i}^{N_c} \sum_{i<j}^{N+c} \frac{1}{|\vec{r}_i - \vec{r}_j|} + \cdots \quad (1)$$

- Ground state energies, Magnetic and spin orders and correlations. Magnetization measurements: SQUID
- Superconducting orders and gaps. Superconducting gaps: Andreev spectroscopy
- $A(k,\omega)$. ARPES measurements
- $N(r,\omega)$. STM measurements
- $S(k,\omega)$. neutron scattering measurements

Defining the Theory Problem

$$H = -\sum_{i=1}^{Nc} \frac{\hbar^2 \nabla^2}{2m_e} + \frac{e^2}{4\pi\epsilon_0} \sum_{i}^{N_c} \sum_{i<j}^{N+c} \frac{1}{|\vec{r}_i - \vec{r}_j|} + \cdots \quad (1)$$

- Ground state energies, Magnetic and spin orders and correlations. Magnetization measurements: SQUID
- Superconducting orders and gaps. Superconducting gaps: Andreev spectroscopy
- $A(k, \omega)$. ARPES measurements
- $N(r, \omega)$. STM measurements
- $S(k, \omega)$. neutron scattering measurements

Defining the Theory Problem

$$H = -\sum_{i=1}^{Nc} \frac{\hbar^2\nabla^2}{2m_e} + \frac{e^2}{4\pi\epsilon_0}\sum_{i}^{N_c}\sum_{i<j}^{N+c}\frac{1}{|\vec{r}_i - \vec{r}_j|} + \cdots \quad (1)$$

- Ground state energies, Magnetic and spin orders and correlations. Magnetization measurements: SQUID
- Superconducting orders and gaps. Superconducting gaps: Andreev spectroscopy
- $A(k,\omega)$. ARPES measurements
- $N(r,\omega)$. STM measurements
- $S(k,\omega)$. neutron scattering measurements

Defining the Theory Problem

$$H = -\sum_{i=1}^{Nc} \frac{\hbar^2 \nabla^2}{2 m_e} + \frac{e^2}{4\pi\epsilon_0} \sum_{i}^{N_c} \sum_{i<j}^{N+c} \frac{1}{|\vec{r}_i - \vec{r}_j|} + \cdots \quad (1)$$

- Ground state energies, Magnetic and spin orders and correlations. Magnetization measurements: SQUID
- Superconducting orders and gaps. Superconducting gaps: Andreev spectroscopy
- $A(k, \omega)$. ARPES measurements
- $N(r, \omega)$. STM measurements
- $S(k, \omega)$. neutron scattering measurements

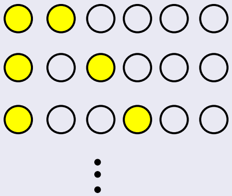
The Exponential Problem in Second Quantization

$$H = \sum_{ij} t_{i,\gamma,j,\gamma'} c^\dagger_{i\gamma} c_{j\gamma'} + \frac{e^2}{4\pi\epsilon_0} \sum_{i}^{N_c} \sum_{i<j}^{N+c} \frac{n_i n_j}{|\vec{r}_i - \vec{r}_j|} + \cdots \qquad (2)$$

The Exponential Problem in Second Quantization

$$H = \sum_{ij} t_{i,\gamma,j,\gamma'} c^{\dagger}_{i\gamma} c_{j\gamma'} + \frac{e^2}{4\pi\epsilon_0} \sum_{i}^{N_c} \sum_{i<j}^{N+c} \frac{n_i n_j}{|\vec{r}_i - \vec{r}_j|} + \cdots \qquad (2)$$

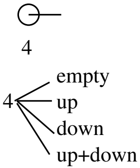
Example: 6 sites, 2 electrons leads to $C^6_2 = 15$ states



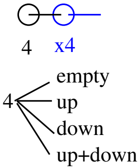
What does exponential mean?

- 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 (!)

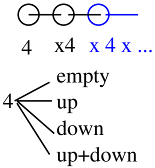
DMRG Basics: Wilson's RG



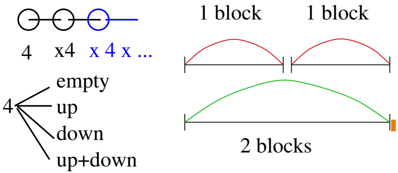
DMRG Basics: Wilson's RG



DMRG Basics: Wilson's RG



DMRG Basics: Wilson's RG



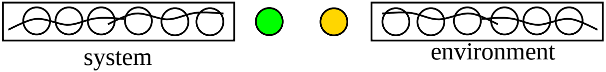
DMRG Basics

- Algorithm: “Density Matrix Renormalization Group” [White, PRL ’92 and PRB ’92]
- Discard (an exponential number of) states. Keep *m* states in Hibert space at all times.
- Controlled error, exponentially decaying with *m* for most 1D systems.

DMRG Basics

- Algorithm: “Density Matrix Renormalization Group” [White, PRL ’92 and PRB ’92]
- Discard (an exponential number of) states. Keep *m* states in Hibert space at all times.
- Controlled error, exponentially decaying with *m* for most 1D systems.

DMRG Basics

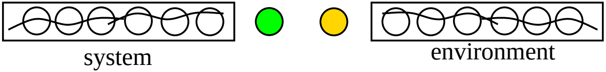


- Algorithm: “Density Matrix Renormalization Group” [White, PRL ’92 and PRB ’92]
- Discard (an exponential number of) states. Keep m states in Hibert space at all times.
- Controlled error, exponentially decaying with m for most 1D systems.

DMRG Basics

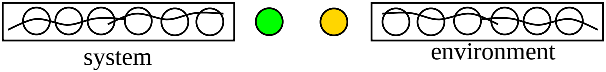
- Algorithm: "Density Matrix Renormalization Group" [White, PRL '92 and PRB '92]
- Discard (an exponential number of) states. Keep m states in Hibert space at all times.
- Controlled error, exponentially decaying with m for most 1D systems.

DMRG Basics



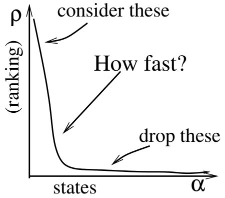
- Algorithm: "Density Matrix Renormalization Group" [White, PRL '92 and PRB '92]
- Discard (an exponential number of) states. Keep *m* states in Hibert space at all times.
- Controlled error, exponentially decaying with *m* for most 1D systems.

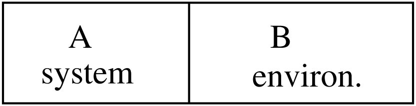
DMRG Basics



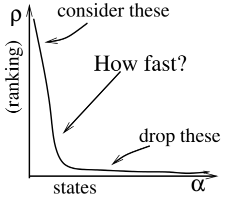
- Algorithm: “Density Matrix Renormalization Group” [White, PRL ’92 and PRB ’92]
- Discard (an exponential number of) states. Keep m states in Hibert space at all times.
- Controlled error, exponentially decaying with m for most 1D systems.

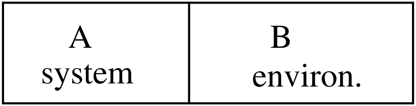
Why does the DMRG work...
...when it does, and doesn't when it doesn't?





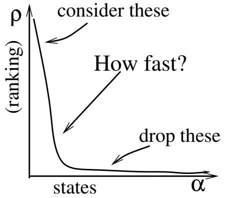
Why does the DMRG work...
...when it does, and doesn't when it doesn't?

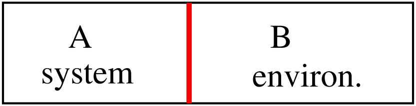




How much entanglement between A and B?

Why does the DMRG work...
...when it does, and doesn't when it doesn't?

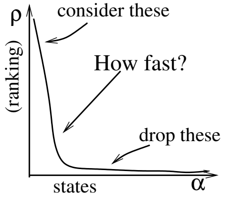


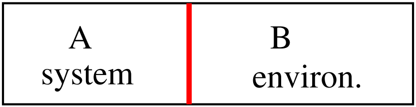


How much entanglement between A and B?

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

Why does the DMRG work...
...when it does, and doesn't when it doesn't?



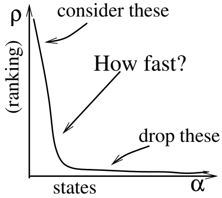


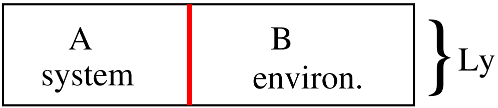
How much entanglement between A and B?

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

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

Why does the DMRG work...
...when it does, and doesn't when it doesn't?





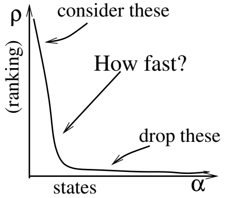
How much entanglement between A and B?

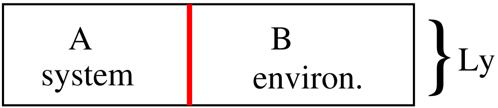
A: Roughly equal to the area between A and B.

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

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

Why does the DMRG work... ...when it does, and doesn't when it doesn't?





How much entanglement between A and B?

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

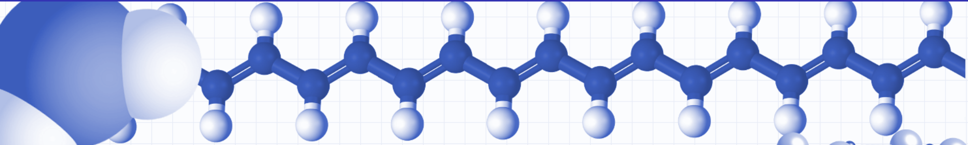
1D: Entropy $\rightarrow S \approx 1 \rightarrow \textit{complexity} = \exp^{S} = \textit{const}.$

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

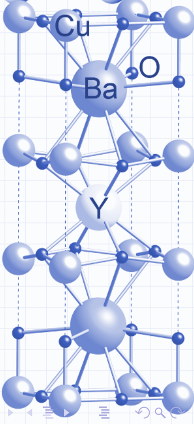
You: Hey! You're handwaving!

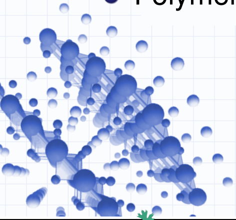
Me: OK, OK, see: [J. Eisert et al., Rev. Mod. Phys., 2010]

Applications of the DMRG



- Spin systems (quantum Heisenberg model, etc.)
- Fermionic systems (Hubbard, t-J, etc.)
- Quantum chemistry,
  [White and Martin, J. Chem. Phys. 1999]
- Polymers, [LetPetit and Pastor, PRB 1997]



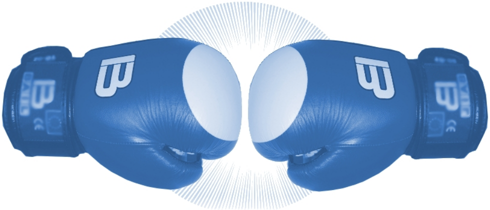


DMRG vs. QMC

Only two non-perturbative methods

Item	**DMRG**	**QMC**
Complexity	Pol. in 1D, Exp. in 2D	Pol., Exp. if SP[a]
Real time and freq.	Yes	No
Finite temperature	Maybe	Yes
Active Research	Yes	Yes

[a] SP stands for Sign Problem



DMRG Topics

- Time
- Temperature
- Dynamics

Time Evolution

- Problem: To compute things like this:
$\langle\phi|e^{iHt}A_{0,\pi(0)}A_{1,\pi(1)}\cdots A_{a-1,\pi(a-1)}e^{-iHt}|\phi\rangle$ with
$|\phi\rangle = B_{b-1,\pi'(b-1)}\cdots B_{1,\pi'(1)}B_{0,\pi'(0)}|\psi\rangle$

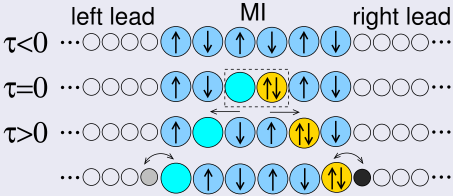
Time Evolution

- Problem: To compute things like this:
  $\langle\phi|\mathrm{e}^{iHt}A_{0,\pi(0)}A_{1,\pi(1)}\cdots A_{a-1,\pi(a-1)}\mathrm{e}^{-iHt}|\phi\rangle$ with
  $|\phi\rangle = B_{b-1,\pi'(b-1)}\cdots B_{1,\pi'(1)}B_{0,\pi'(0)}|\psi\rangle$
- Solution: To target multiple states, like $\exp(iHt)\cdots|\phi\rangle$

Time Evolution

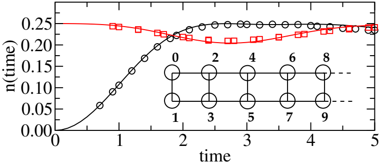
- Problem: To compute things like this:
  $\langle\phi|e^{iHt}A_{0,\pi(0)}A_{1,\pi(1)}\cdots A_{a-1,\pi(a-1)}e^{-iHt}|\phi\rangle$ with
  $|\phi\rangle = B_{b-1,\pi'(b-1)}\cdots B_{1,\pi'(1)}B_{0,\pi'(0)}|\psi\rangle$
- Solution: To target multiple states, like $\exp(iHt)\cdots|\phi\rangle$

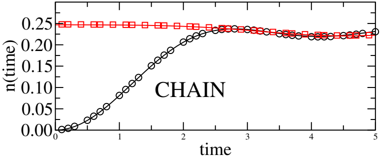
Time propagation of an electronic excitation

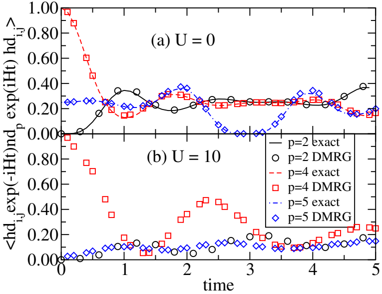


[From L.G.G.V. Dias Da Silva et al., PRB 2010]

Time Evolution: Accuracy





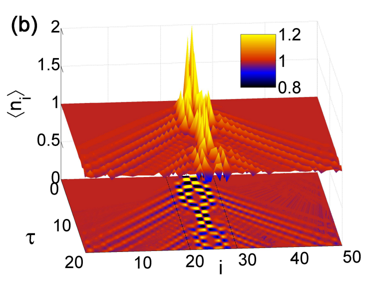


[Alvarez et al, http://arxiv.org/abs/1103.5391]

Time Evolution: Mott Insulators for Solar Cells[1]

Our theory work:

Past: [Dias Da Silva, PRB 2010]

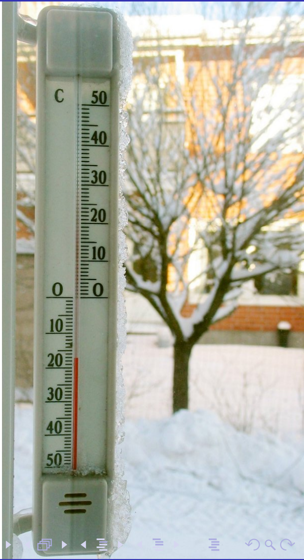


Present: Layered geometries

[1] See [E. Manousakis, PRB 2010] for a review and references therein

DMRG Topics

- Time
- Temperature
- Dynamics



Temperature $T = 1/\beta$

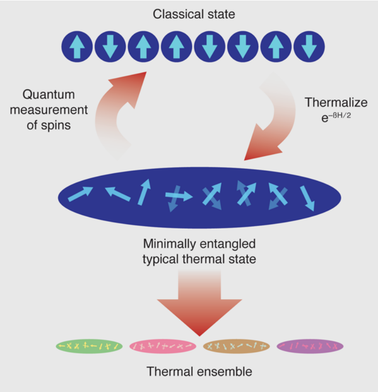
- Problem: At $T > 0$ mixing of states leads to entanglement. $Z = \sum_E \exp(-\beta E)|E\rangle\langle E|$

Temperature $T = 1/\beta$

- Problem: At $T > 0$ mixing of states leads to entanglement. $Z = \sum_E \exp(-\beta E)|E\rangle\langle E|$
- Old solution: Purify states...too costly [todo: Add reference here]

Temperature $T = 1/\beta$

- Problem: At $T > 0$ mixing of states leads to entanglement. $Z = \sum_E \exp(-\beta E)|E\rangle\langle E|$
- Old solution: Purify states...too costly [todo: Add reference here]
- New Solution: Minimally entangled typical thermal states (METTS) [S. R. White, PRL 2009]

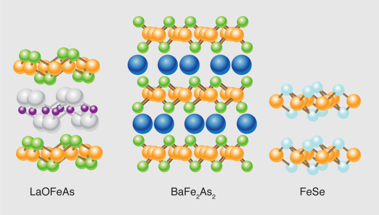


[U. Schollwöck, Physics 2, 39 (2009)]

Application: Iron Pnictides Superconductors

Why Fe-based superconductors?

Because spin flipping terms in Hamiltonian make it difficult for quantum Monte Carlo

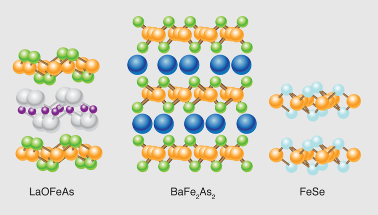


[from M. Johannes, Physics 2008]

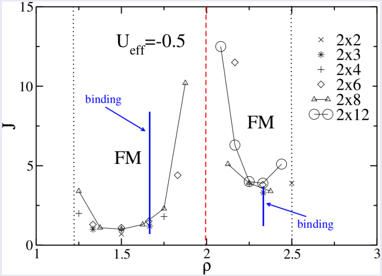
Application: Iron Pnictides Superconductors

Why Fe-based superconductors?

Because spin flipping terms in Hamiltonian make it difficult for quantum Monte Carlo



[from M. Johannes, Physics 2008]

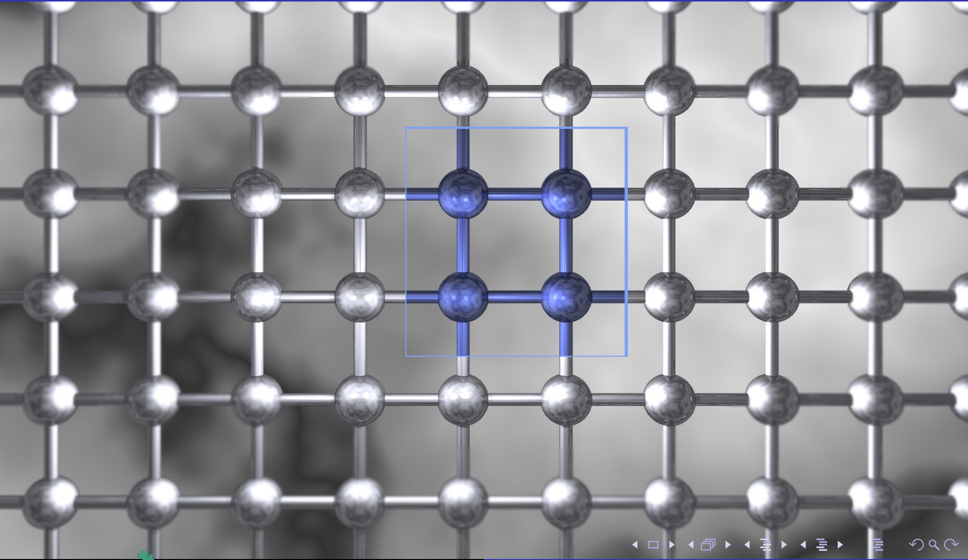


[from CNMS user project, Xavier et al., PRB 2010]

DMRG Topics

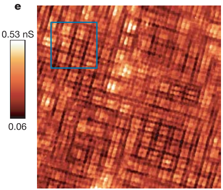
- Time
- Temperature
- Dynamics

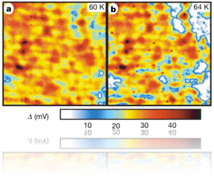
Dynamics: Use DMRG as an cluster solver

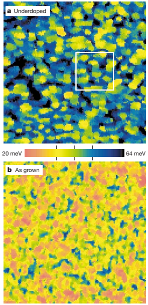


Emergence: Electronic Inhomogeneities in Cuprates

- Spin and charge stripes, [Tranquada et al., '95; Mook et al., '00]
- Checkerboard charge modulations, [Hanaguri, Davis et al., '04]
- Random superconducting gap modulations, [Lang, Davis eta l., '02; Gomes, Yazdani et al., '07]







Emergence: Caution: Philosophy ahead

Emergence: Tigers are real[2]

An emerging object

- ~~Reductionism~~
- ~~Fuzziness (not well defined)~~
- Independent reality instead

[2] [From D. Wallace, Decoherence and Ontology, in Saunders, Barrett, Kent, and Wallace (ed.), Many Worlds? Everett, Quantum Theory, and Reality, Oxford University Press, Oxford, 2010]

Summary

Our Interests and Future Research

- DMRG: Time: http://arxiv.org/abs/1103.5391
- DMRG: Temperature
  http://physics.aps.org/articles/v2/39
- DMRG: Dynamics DMRG as an cluster solver

Thanks to:

E. Dagotto, L. Dias da Silva, P. Kent, T. Maier, S. Manmana, E. Stoudenmire, M. Simonson, M. Summers, J. Xavier
Thanks to: The DOE Early Career Research Program, and the Office of Science at DOE

Credit Line

This work was supported by the Center for Nanophase Materials Sciences, sponsored by the Scientific User Facilities Division, Basic Energy Sciences, U.S. Department of Energy, under contract with UT-Battelle. This research used resources of the National Center for Computational Sciences, as well as the OIC at Oak Ridge National Laboratory. G.A. acknowledges support from the DOE Early Career Research Program.

Image and Software Credits

Images:
Pavel Sevela / Wikimedia Commons,
http://commons.wikimedia.org/wiki/File:Red_boxing_glove.jpg;
http://commons.wikimedia.org/wiki/File:Pnictide_cristallographic_structure.jpg;
http://commons.wikimedia.org/wiki/File:Polyacetylene-3D-balls.png;
http://commons.wikimedia.org/wiki/File:YBCO-unit-cell-CM-3D-balls-labelled.png;
http://commons.wikimedia.org/wiki/File:Water_molecule.svg;
http://commons.wikimedia.org/wiki/File:Taschenuhr_K-0550.jpg;
Solar panel image thanks to Joy Anderson (ORNL Media).
http://commons.wikimedia.org/wiki/File:Pakkanen.jpg;
http://commons.wikimedia.org/wiki/File:KunioniuMiskas001.JPG;

Software: pdfLaTeXwith beamer package. Gimp. Inkscape. Povray. Xfig. Xmgrace