Computing Correlated Electrons: Roadmap and Roadblocks

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Oak Ridge National Laboratory

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1. The RoadBlocks: Motivation, Problems and Solutions
2. The Roadmap: Time, Temperature, and Dynamics

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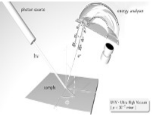
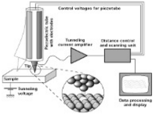
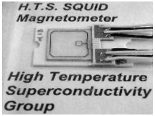
2. The Roadmap: Time, Temperature, and Dynamics
3. The Road Ahead: Computation and Our Strategic Vision

Experiment and Theory

Experiment







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

Theory

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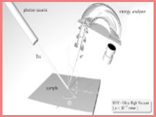
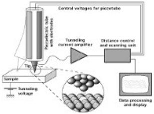

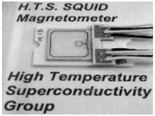

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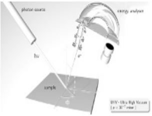

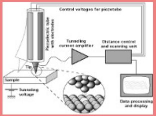

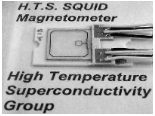

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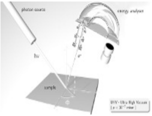

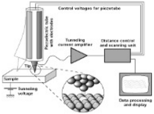

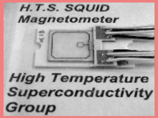

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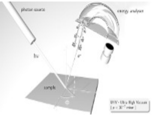

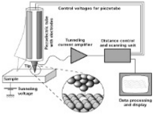

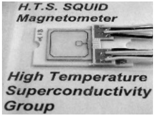

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Theory

Atoms and Electrons

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Atoms and Electrons

Electrons in Matter are often easy to study. . .

But not always.

Some materials are difficult to study
For example,

- superconductors
- magnetic materials,
- quantum dots
- nanostructures with transition metal oxides.

They are also technologically useful.

How do electron correlations cause functionality?

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

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

* See Dagotto, 2005.

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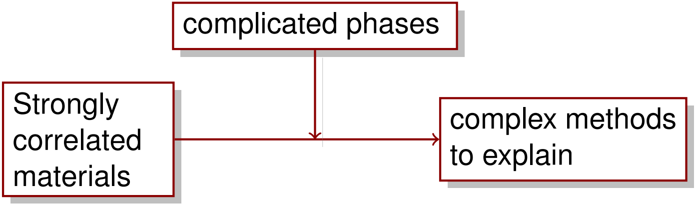

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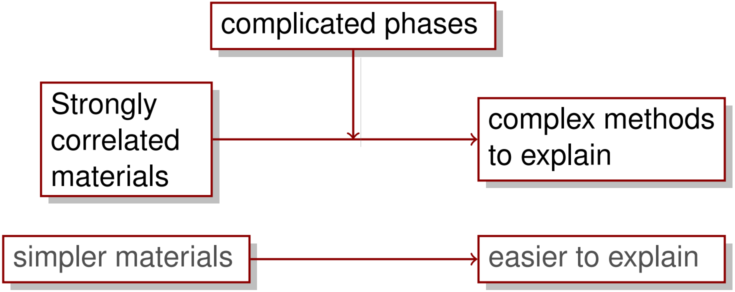

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Therefore, an accurate approach to study strongly correlated materials is needed.

And accurate approaches are costly.

The Exponential Problem in Second Quantization

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

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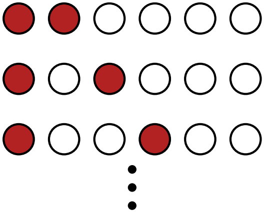
Example: 6 sites, 2 electrons leads to $C_2^6 = 15$ states



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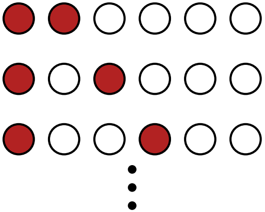

For large N we have Stirling's approximation

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

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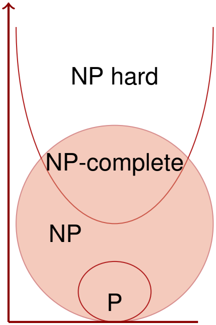
- Problem not even in NP...

Hamiltonian Complexity: Not even in NP!

- NP problems are problems where a solution can be verified in polynomial time.



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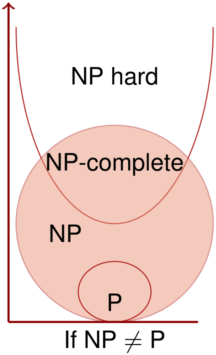
- Given $\vec{v}$ one cannot verify in polynomial time if it's an eigenvector of H. . . . Because H has rank exponential in the number of sites.



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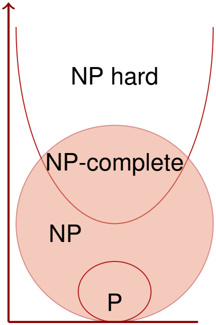
- Given $\vec{v}$ one cannot verify in polynomial time if it's an eigenvector of H.... Because H has rank exponential in the number of sites.
- The Hamiltonian problem is in class Quantum Merlin Arthur*



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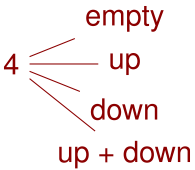
*See Schuch et al., 2008 Schuch and Verstraete, 2009 Cubitt and Montanaro, 2013 Osborne, 2013 Liu et al., 2007 Aharonov and Naveh, 2002

Renormalization Group



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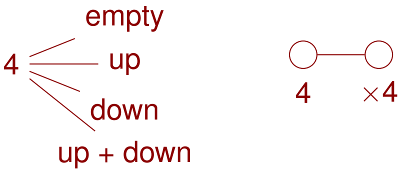

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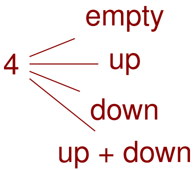

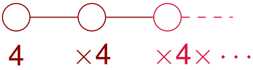

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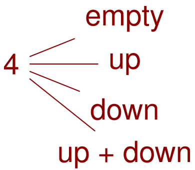
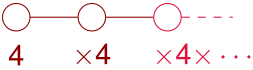
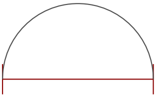




1 block



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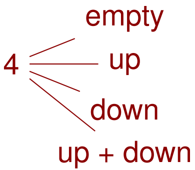

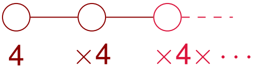

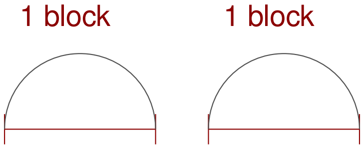

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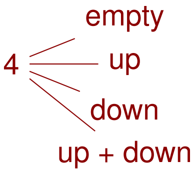

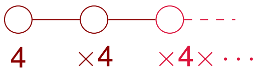

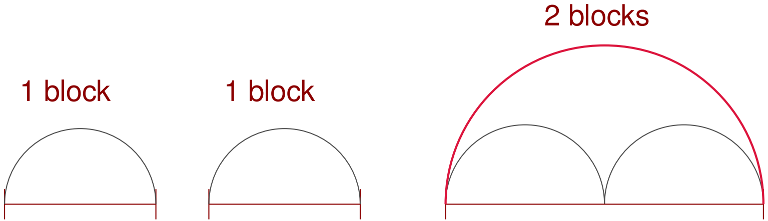

Density Matrix Renormalization Group

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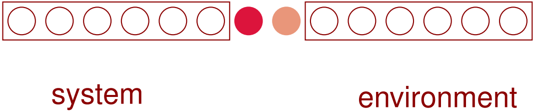

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- Discard (an exponential number of) states. Keep m states in Hibert space at all times.

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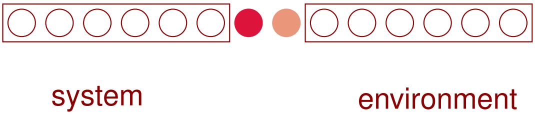
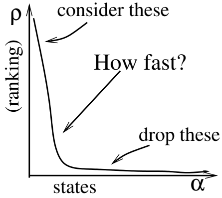
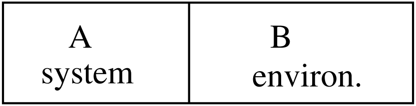


- Discard (an exponential number of) states. Keep *m* states in Hibert space at all times.
- Controlled error, exponentially decaying with *m* for most 1D systems.

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





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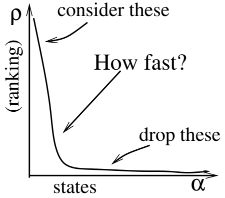

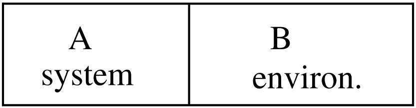

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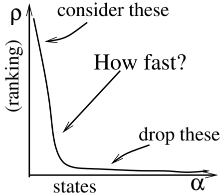

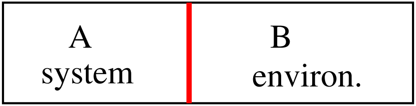

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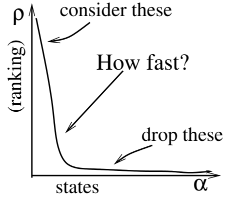

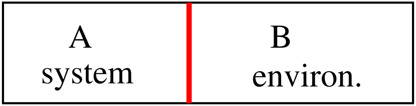

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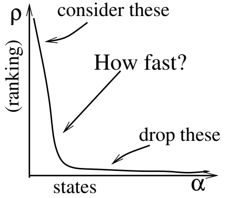

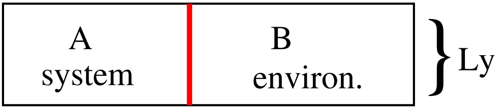

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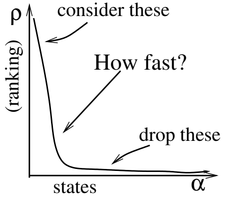

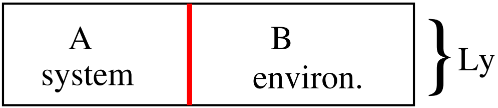

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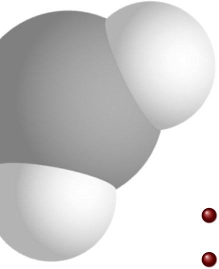
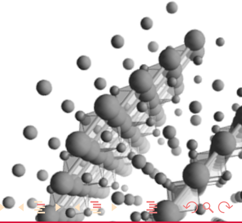
2D: Entropy $\to S \approx L_y \to$ *complexity* $= \exp^{L_y} =$ *exponential*

You : Hey! You're handwaving!
Me : OK, OK, see: Eisert et al., 2010

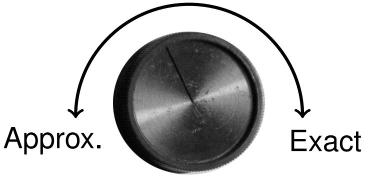
Applications of the DMRG



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

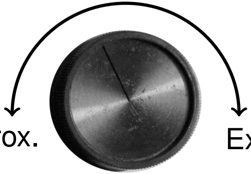


Only Two Methods: DMRG and QMC



Method must become exact systematically

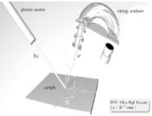
Only Two Methods: DMRG and QMC

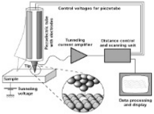


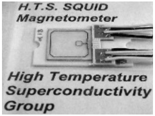
Method must become exact systematically

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

*SP stands for Sign Problem







1. The RoadBlocks: Motivation, Problems and Solutions
2. **The Roadmap: Time, Temperature, and Dynamics**
3. The Road Ahead: Computation and Our Strategic Vision

Roadmap: Time, Temperature, and Dynamics

- Time
- Temperature
- Dynamics

Time Evolution: Mott Insulators for Solar Cells

Time Evolution: Mott Insulators for Solar Cells

Time propagation of an electronic excitation

left lead MI right lead

$\tau < 0$ $\cdots \circ\circ\circ\circ \uparrow\downarrow\uparrow\downarrow\uparrow\downarrow \circ\circ\circ\circ \cdots$

Time Evolution: Mott Insulators for Solar Cells

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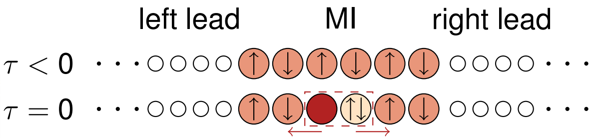

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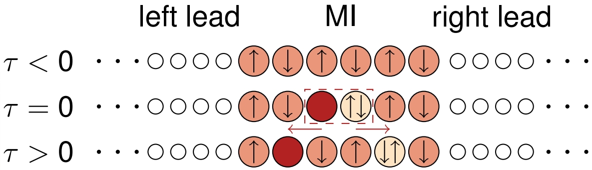

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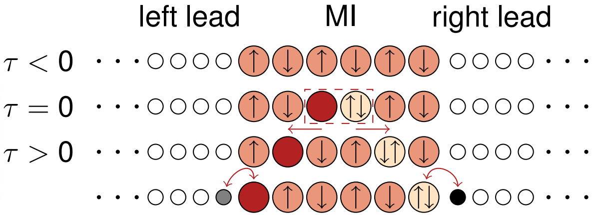

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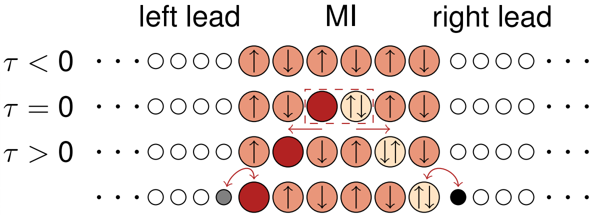

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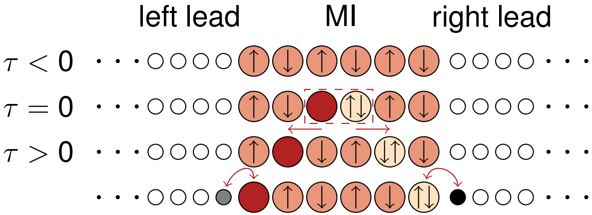

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For a review see Manousakis, 2010 and references therein

We use Krylov-space Time Evolution

Tridiagonalize $H = V^\dagger T V$ starting Lanczos with $|\phi\rangle$.
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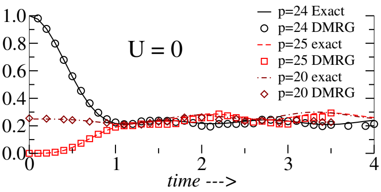
* This is within a DMRG method, so don't forget to target the appropriate states. For an implementation, see Alvarez et al., 2011.

Time Evolution: Our Theory Work

Accuracy of tDMRG



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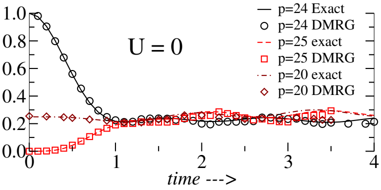

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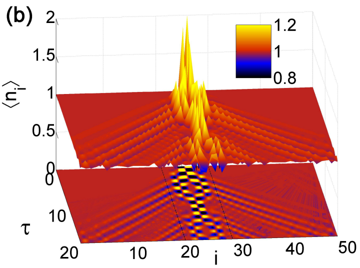
Propagation of a holon-doublon



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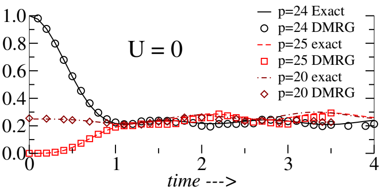

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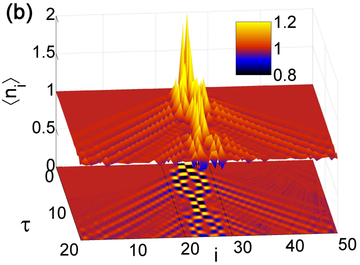

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For our theory work on time evolution, see also
da Silva et al., 2012, da Silva et al., 2013, Al-Hassanieh et al., 2013.

Time, Temperature, and Dynamics

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

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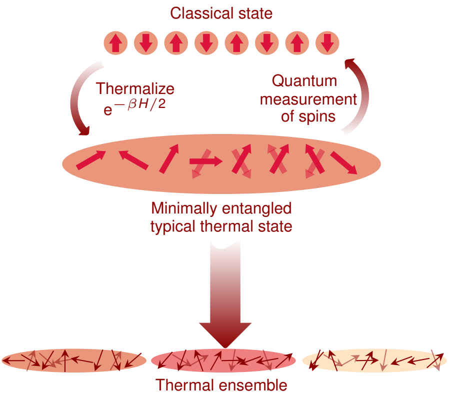
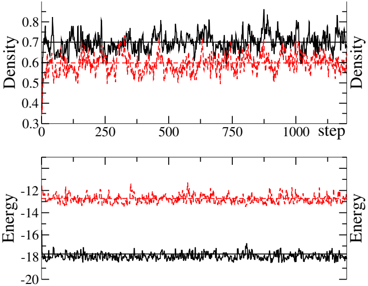


Adapted from Schollwöck, 2009

Temperature Dependence: Our Work

$$H = \sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i,\sigma} V_i n_{i,\sigma},$$



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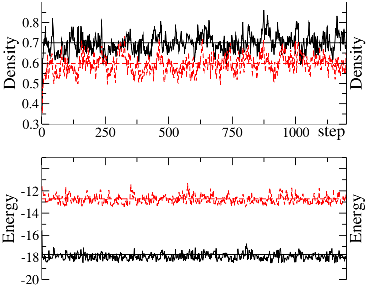

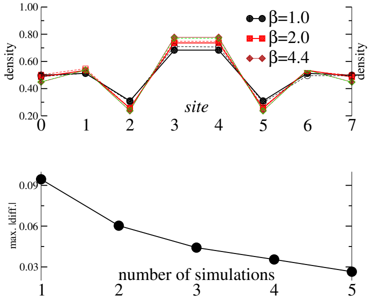

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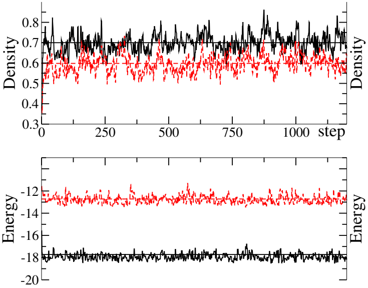

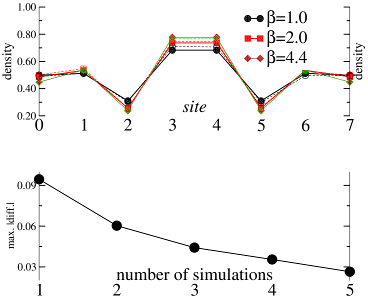

Both figures are from Alvarez, 2013.

Talk Tomorrow Afternoon. Q46.6

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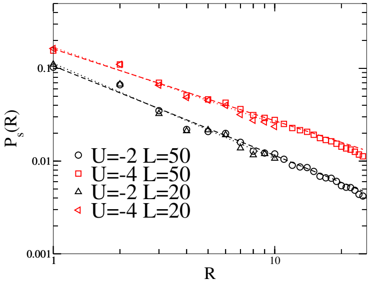
$$H = \sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \mu \hat{N}$$



Hubbard chain with length L (as indicated) for $T = 0$.

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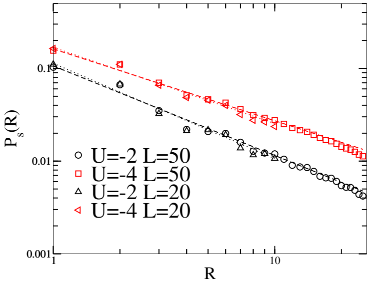

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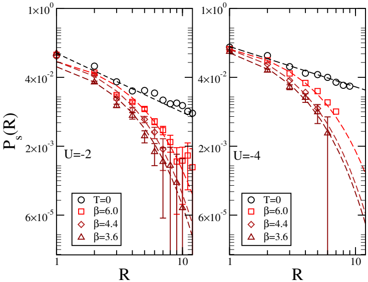

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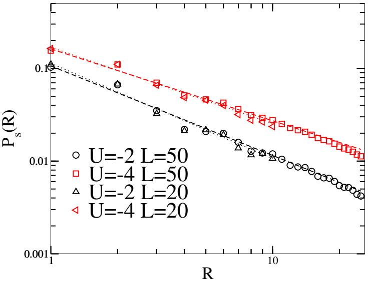

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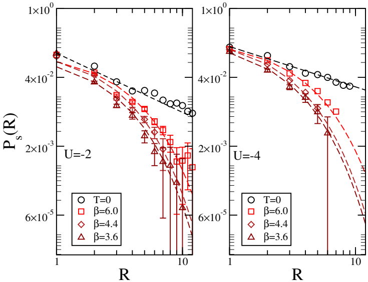

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Talk Tomorrow Afternoon. Q46.6

Time, Temperature, and Dynamics

- Time
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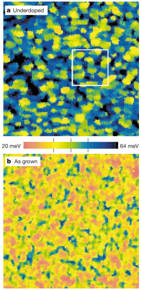
- Other methods. Active area of research
  Jeckelmann, 2002, Dargel et al., 2011, Dargel et al., 2012.

Nanoscale Emergent Electronic Patterns in Cuprates

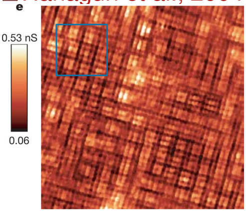
Spin and charge stripes

Tranquada et al., 1995, Mook et al., 2002



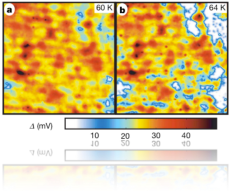
Checkerboard charge modulations

Hanaguri et al., 2004

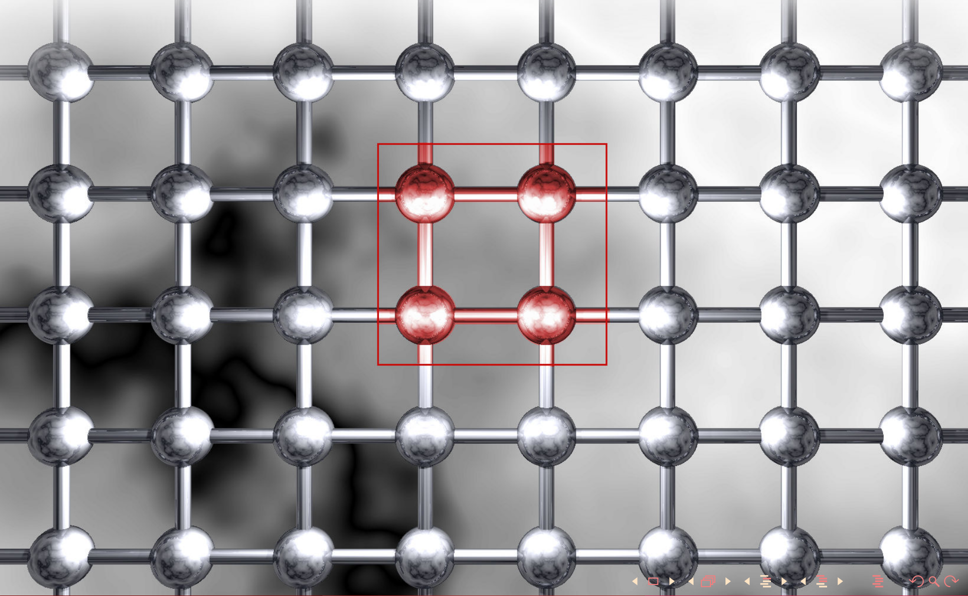


Random superconducting gap modulations

Lang et al., 2002



DMRG as an “impurity” solver



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- Let us not throw it over the wall:
    - Software available at `github.com`
    - Same code I use
    - Updates don't break what works

High Performance Computing

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- But hardware landscape (GP-GPUs) is challenging given our aims

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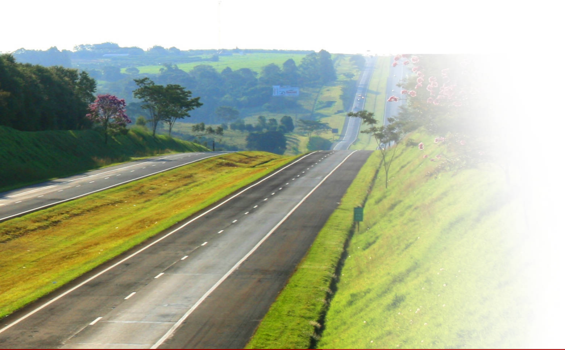
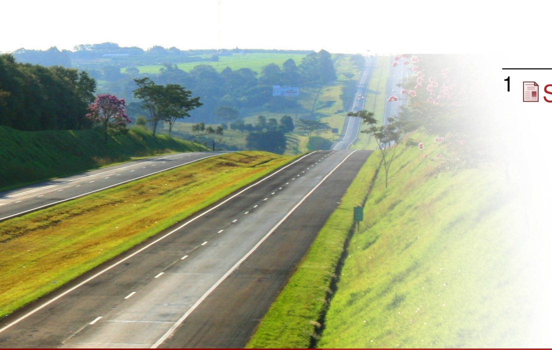
The Road Ahead: Our Strategic Vision



The Road Ahead: Our Strategic Vision

- Implement parallel DMRG[1]



[1] Stoudenmire and White, 2013

The Road Ahead: Our Strategic Vision

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- Implement parallel DMRG[1]
- Work towards 2D DMRG
- Develop a matrix product states code
- Stay at the vanguard of renormalization methods[2]

1 Stoudenmire and White, 2013
2 Corboz and Vidal, 2009, Evenbly and Vidal, 2009, Koenig et al., 2009, M. Aguado, 2008 M. Rizzi, 2008, Pfeifer et al., 2009, Vidal, 2008, Barthel et al., 2009, Kraus et al., 2010

Opportunities at ORNL

- Diversity in Recruiting Efforts at ORNL
- RAMS (Research Alliance in Mathematics and Science)
- GEM (Graduate Education for Minorities)

Summary: Our Aims

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DMRG++: https://web.ornl.gov/~gz1/dmrgPlusPlus/
Free and open source codes for DMRG, Lanczos, FreeFermions, and spin-phonon fermion models: https://web.ornl.gov/~gz1/
This talk is at https://web.ornl.gov/~gz1/talks/

Credit Line

Thanks to:

K. Al-Hassanieh, E. Dagotto, L. Dias da Silva, P. Kent, T. Maier, S. Manmana, E. Stoudenmire, J. Rincón, M. Summers, S. R. White.

Credit Line

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