Leibniz Universität Hannover

# Introduction to the density-matrix renormalization group

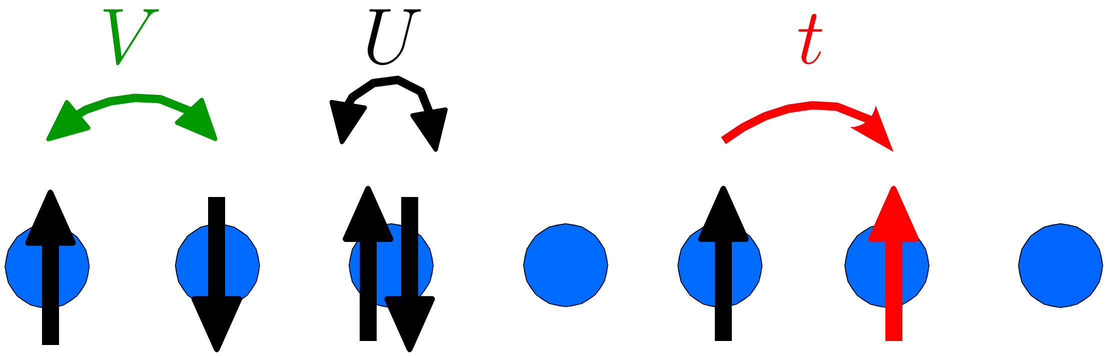
Eric Jeckelmann

Institute for Theoretical Physics
University of Hanover
Germany

# Outline

1. Introduction
2. Density-matrix renormalization group (DMRG):
   Basic principle
3. DMRG code
4. DMRG truncation errors
5. Extension to two-dimensional systems
6. Overview of other extensions
   (TMRG, dynamics, bosons, non-local systems)
7. Conclusion

# Extended one-dimensional Hubbard model




Electronic density

$$0 < \rho < 2$$

## Hamiltonian

$$\hat{H} = -t\sum_{i\sigma}\left(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i+1\sigma} + \hat{c}^{\dagger}_{i+1\sigma}\hat{c}_{i\sigma}\right) - t'\sum_{i\sigma}\left(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i+2\sigma} + \hat{c}^{\dagger}_{i+2\sigma}\hat{c}_{i\sigma}\right)$$
$$+U\sum_{i}\left(\hat{n}_{i\uparrow} - \frac{\rho}{2}\right)\left(\hat{n}_{i\downarrow} - \frac{\rho}{2}\right) + V\sum_{i}(\hat{n}_i - \rho)(\hat{n}_{i+1} - \rho)$$

# Quantum many-body problem

- Physical properties for a N-site lattice ?

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \;, \qquad H\psi = E\psi \;, \qquad Z = Tr\,\exp(-\beta H)$$

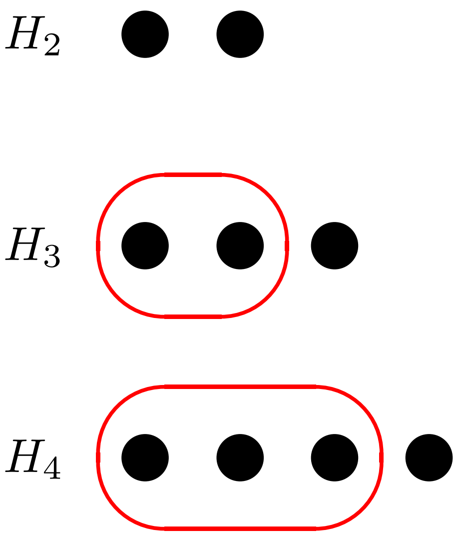
- Exact analytical results for special cases only
  (for instance, 1D Hubbard model, Tomonaga-Luttinger model).

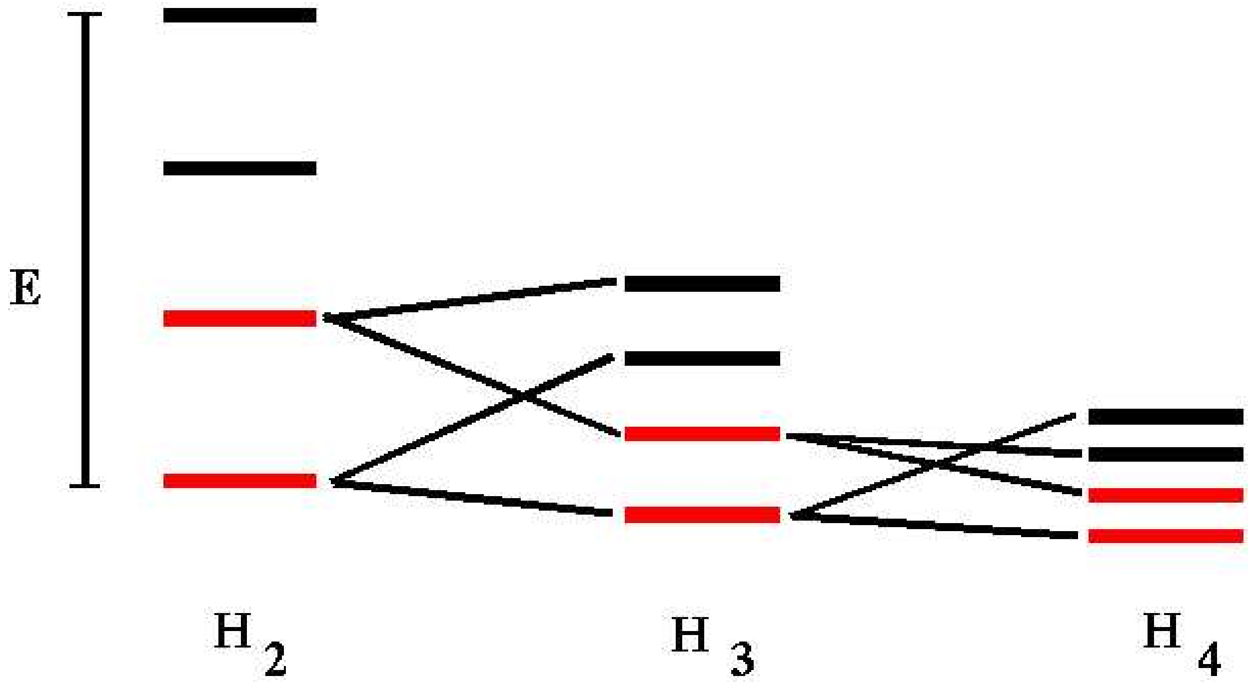
- Hilbert space dimension $= 4^N$
  $\Rightarrow$ Exact diagonalizations up to $N \approx 16$ only.

- "Exact" numerical methods for $N \gg 1$ ?

# Numerical renormalization group (NRG)

**[K.G. Wilson, Rev. Mod. Phys. 47, 773 (1975)]**

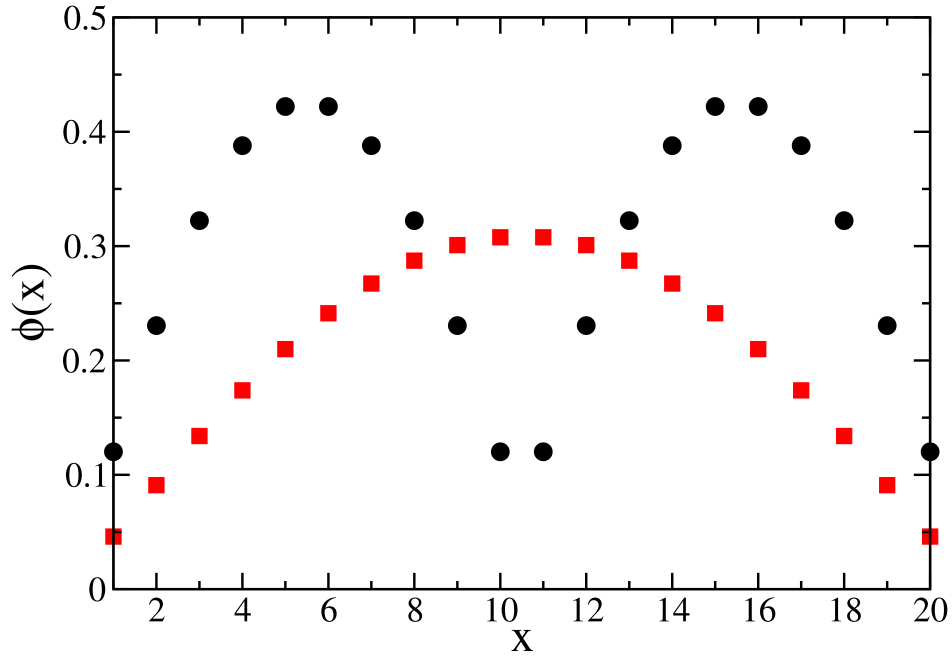


# NRG for the particle-in-the-box problem

[S.R. White and R.M. Noack, PRL **68**, 3487 (1992)]

$$H = -\sum_{i=1}^{L-1} \left( |i\rangle\langle i+1| + |i+1\rangle\langle i| \right) + 2\sum_{i=1}^{L} |i\rangle\langle i| \;\approx\; -\frac{d^2}{dx^2}$$



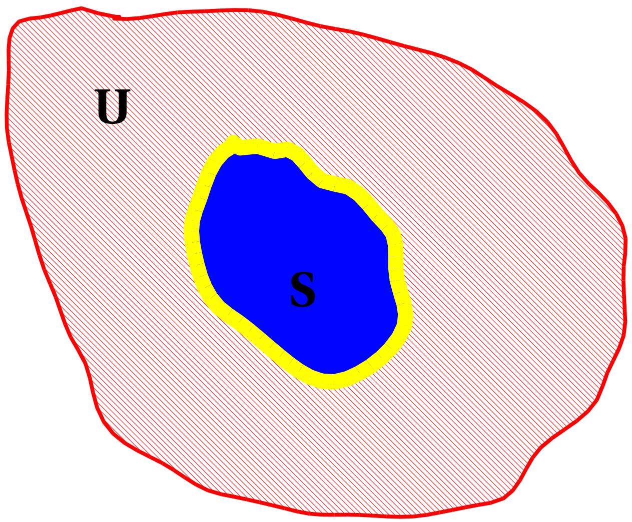

**Lowest eigenstates (L=10,20)**

$$|2L\rangle \neq |L\rangle \otimes |L\rangle$$

**Low-energy states of system $\neq$ Low-energy states of subsystems**

# Reduced density matrix

**System + Environment**




$$|\psi\rangle = \sum_{i,\alpha} \psi_{i,\alpha} \, |i\rangle_S \, |\alpha\rangle_E$$

$$\rho_{i,j} = \sum_\alpha \psi_{i,\alpha} \psi^*_{j,\alpha}$$

$$\sum_j \rho_{i,j} \phi_{\mu,j} = \lambda_\mu \phi_{\mu,i}$$

$$H = H_S + H_E + H_{SE}$$

$$0 \le \lambda_\mu \le 1 \quad \sum_\mu \lambda_\mu = 1$$

**The most important states for the system are**

$$|\phi_\mu\rangle_S = \sum_i \phi_{\mu,i} |i\rangle_S$$

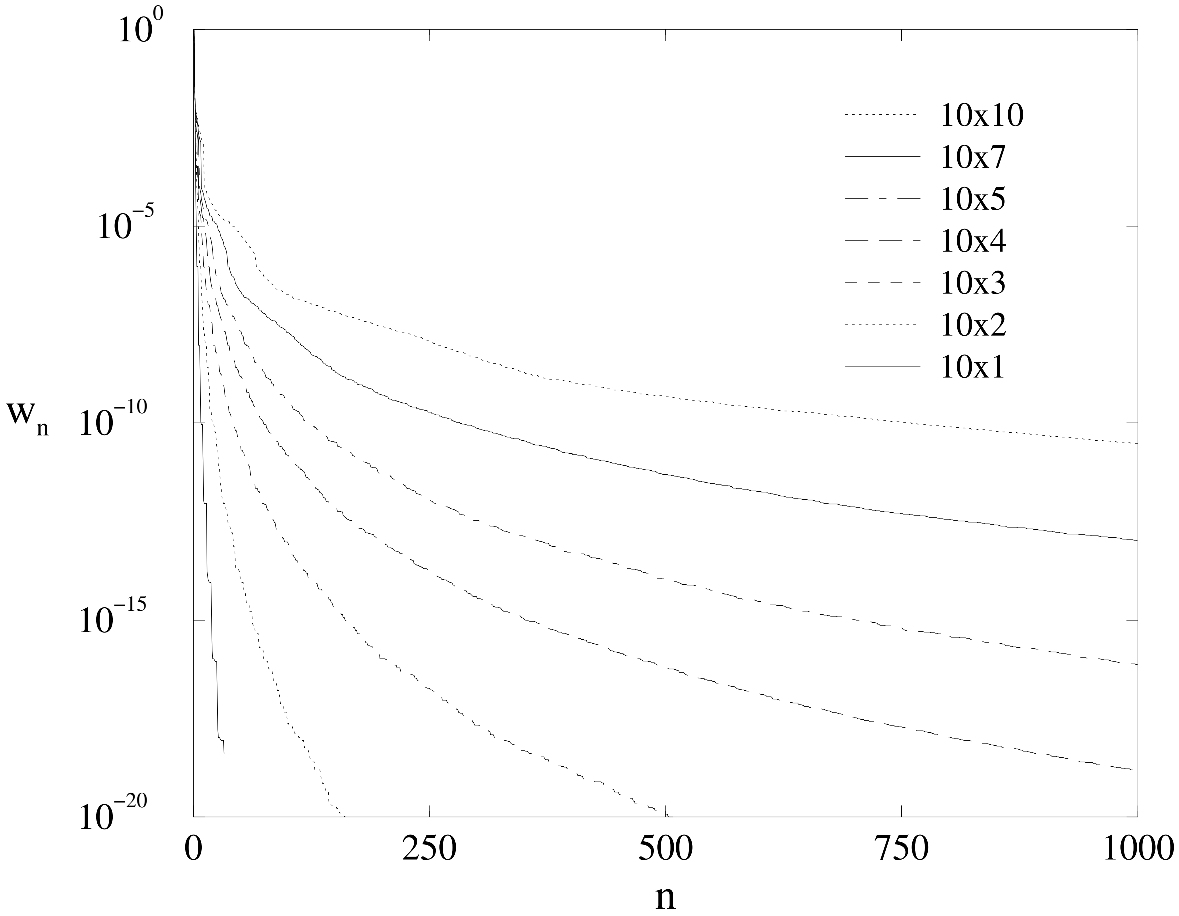
**for the largest density-matrix eigenvalues** $\lambda_\mu$

# Density-matrix eigenvalues

Gapped system of interacting harmonic oscillators
[M. C. Chung and I. Peschel, Phys. Rev. B **62**, 4191 (2000)]

$$w_n \sim \exp\left(-(\text{const.}/N)\ln^2(n)\right)\ , \quad N = \textbf{number of chains}$$

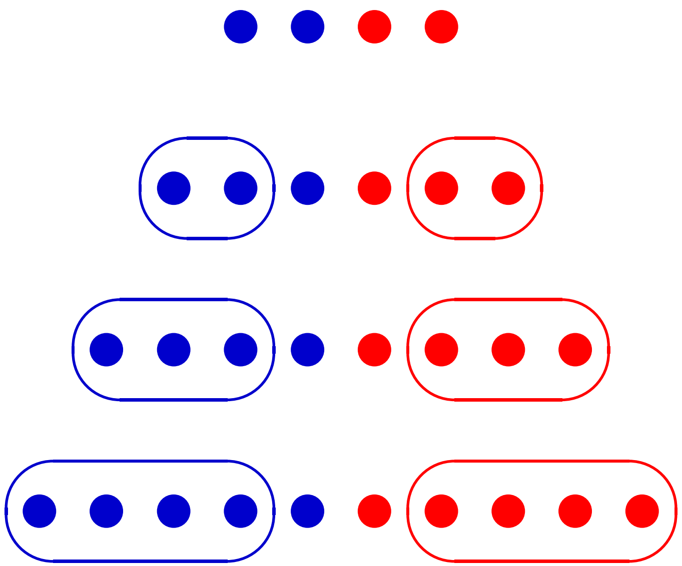
[Generalization of K. Okunishi, Y. Hieida, and Y. Akutsu, Phys. Rev. E **59**, R6227 (1999)]



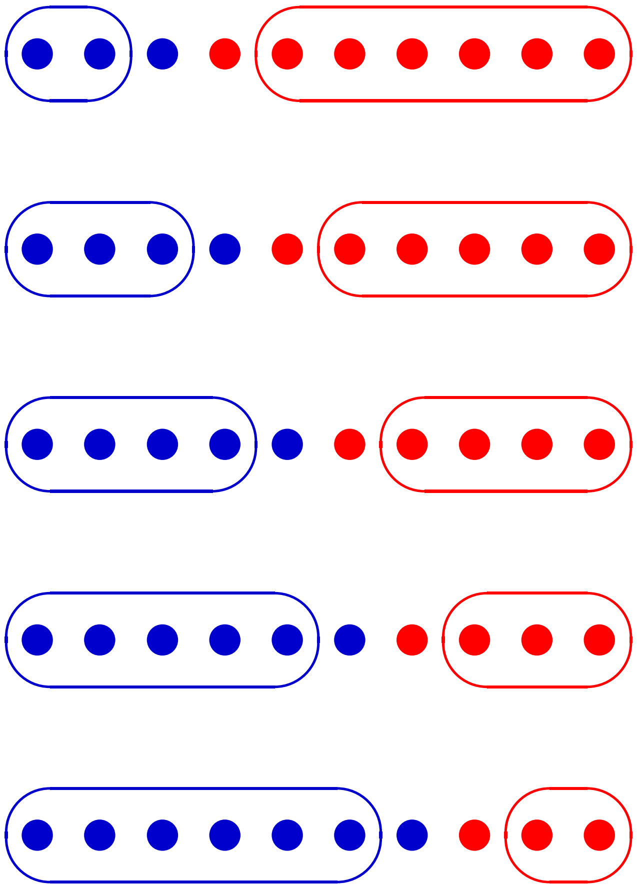
# Density-matrix renormalization group (DMRG)

[S.R. White, PRL **69**, 2863 (1992); PRB **48**, 10345 (1993)]

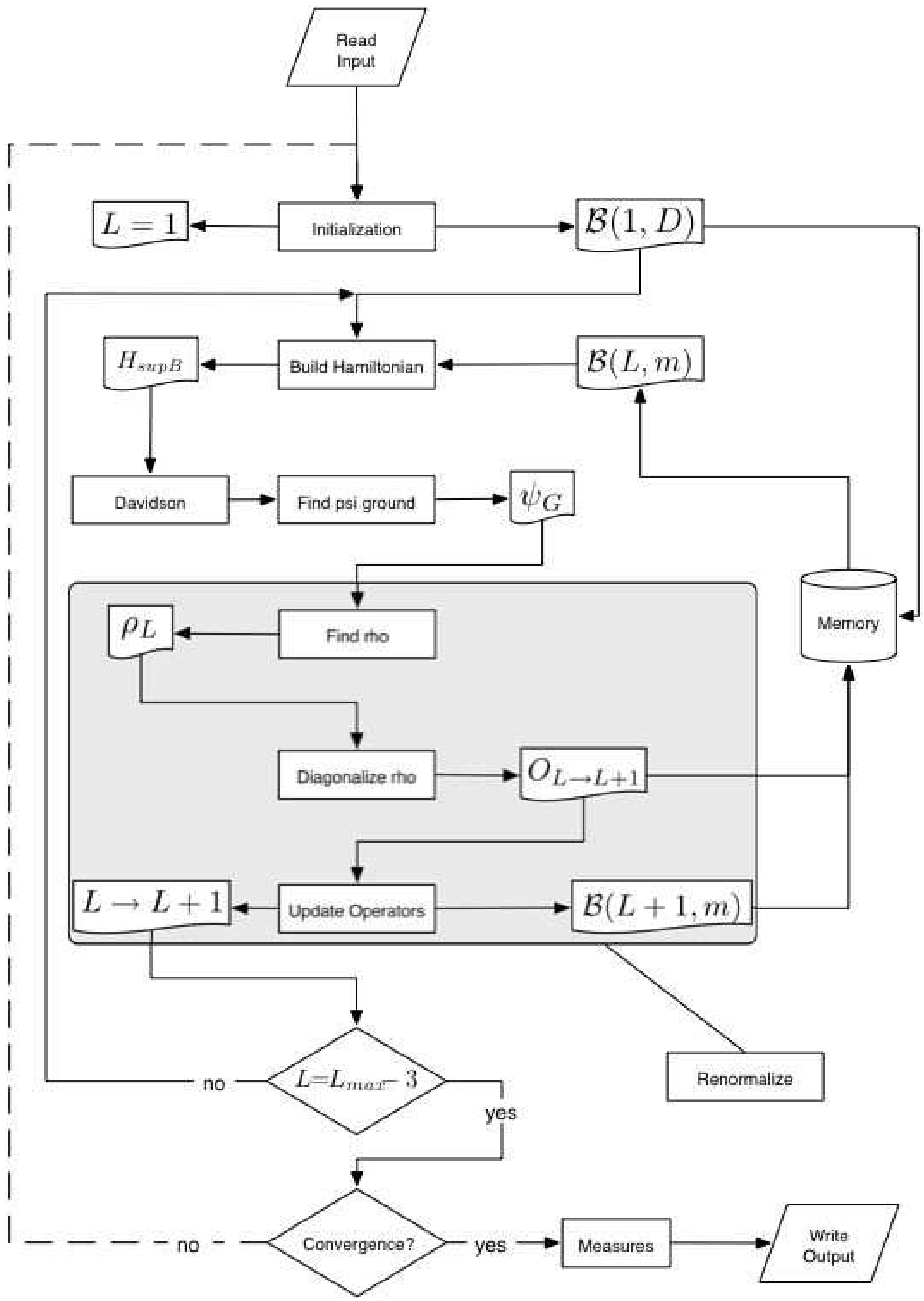
## Infinite system



## Finite system



# DMRG code




From De Chiara *et al.*,
e-print arXiv:cond-mat/0603842

Open source code (FORTRAN90)
available at
http://qti.sns.it/dmrg/phome.html

# Optimization of DMRG calculations

1. Efficient iterative algorithms for superblock calculations (Lanczos or Davidson algorithms, conjugate gradient, ...)

2. Use symmetries and quantum number conservation (block matrix) and/or sparse matrix techniques
   [S. Ramasesha *et al.*, Phys. Rev. B **54**, 7598 (1996);
   I. McCulloch and M. Gulácsi, Europhys. Lett. **57**, 852 (2002)]

3. Use the wavefunction transformation technique
   [S.R. White, Phys. Rev. Lett. **77**, 3633 (1996)]

4. Efficient dynamical memory management (cache, main memory, hard disk)

5. Parallelization
   [G. Hager, E. Jeckelmann, H.Fehske, and G. Wellein, J. Comp. Phys. **194**, 795 (2004)]

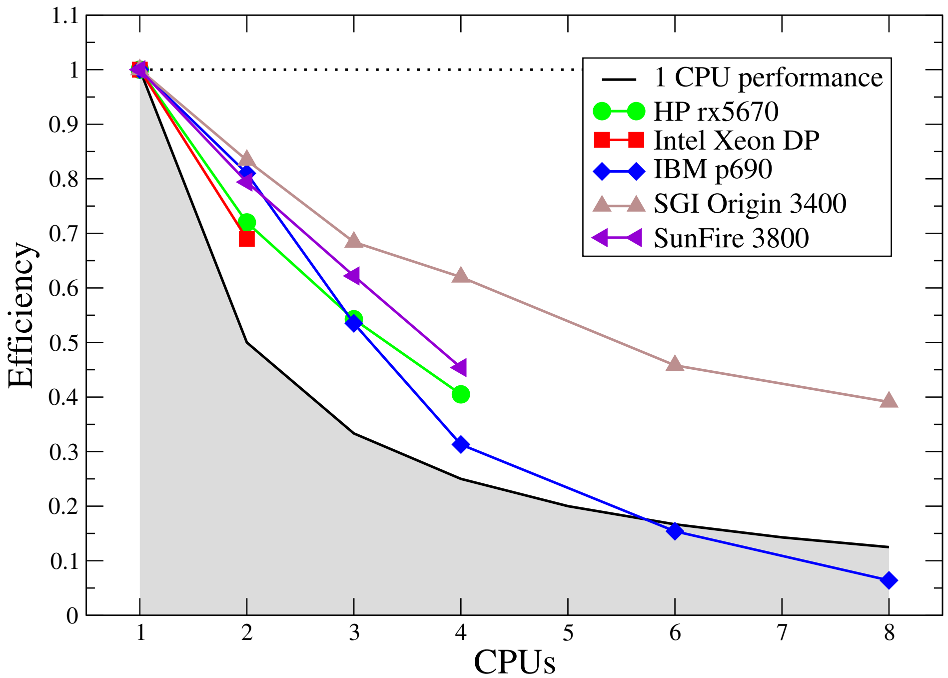
**Overall speedup** $\sim 10^3$

# DMRG code parallelization

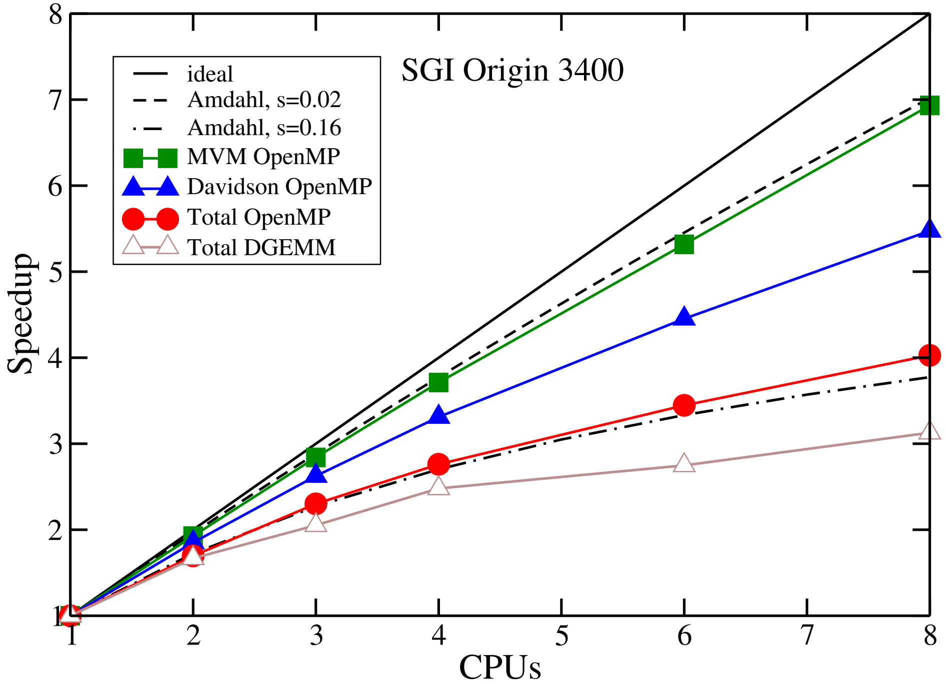
Hager, Jeckelmann, Fehske, Wellein, J. Comp. Phys. 2004

- Single-CPU performance = 40-80% of system peak performance
- Shared-memory parallelization of BLAS DGEMM (dense matrix multiplications)
- OpenMP parallelization of sparse matrix-vector multiplications (MVM) $\psi' = H\psi$

## Benchmarks for $m = 2000$ (Hubbard model)




DGEMM parallelization




MVM parallelization

# Numerical errors

**Superblock calculations with iterative procedures**
(Lanczos or Davidson algorithms, conjugate gradient)

**Convergence (self-consistence) of DMRG basis**

$\mathcal{R}[\rho] = \rho$ for all density matrices $\rho$

**Truncation errors**

Discarded weight (of density matrix $\rho$): $P_m = 1 - \sum_{k=1}^{m} \lambda_k$

Scaling $\quad \Delta\langle H \rangle \sim P_m \quad$ and $\quad \Delta\langle \mathcal{O} \rangle \sim \sqrt{P_m}$

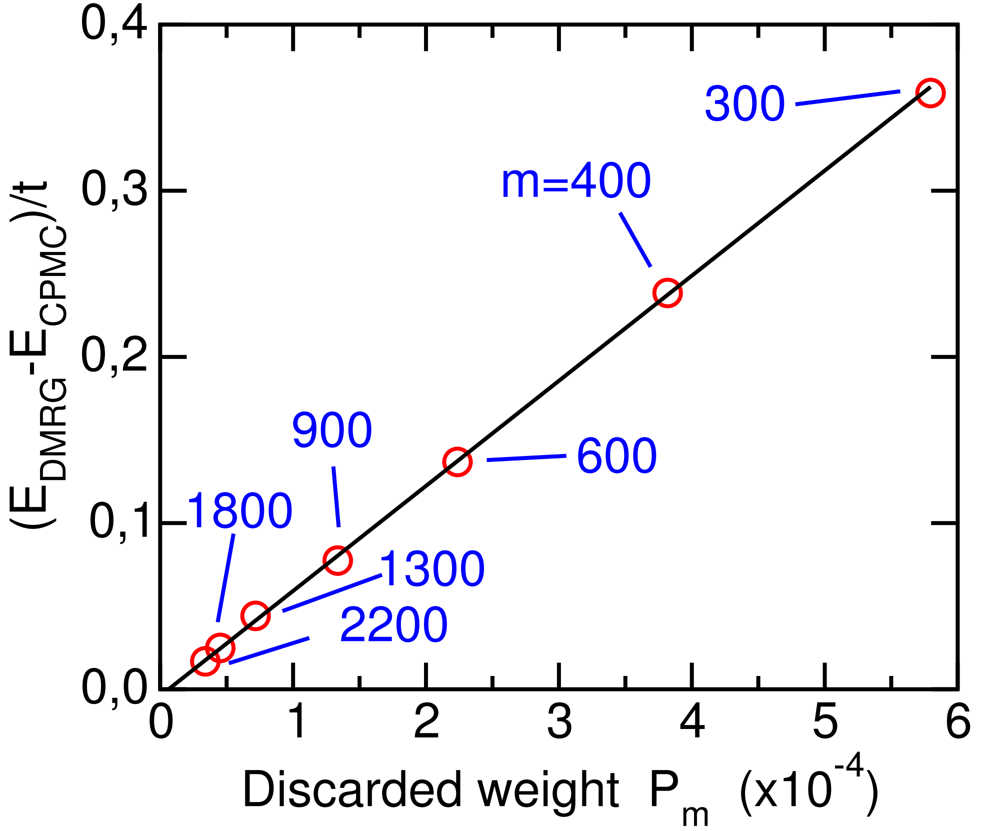
(Exact diagonalization for $P_m \to 0$)

**Finite-size effects**
(Boundary conditions, discrete spectrum)

# DMRG truncation error

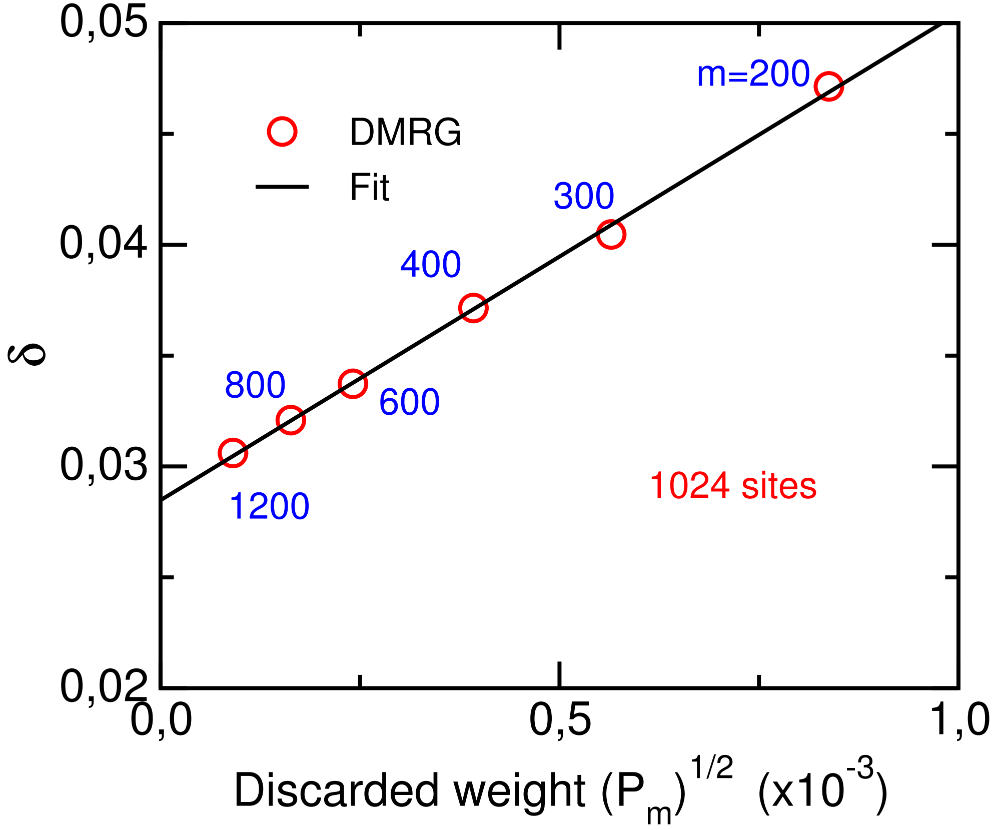
## Energy vs. discarded weight

12x3 Hubbard ladder, U=t, 6 holes




## Staggered bond order vs discarded weight

Half-filled extended Hubbard model, U=3t, V=1.5t




$$E_m = E_{\mathrm{exact}} + cP_m$$

$$\delta = \delta_{\mathrm{exact}} + c\sqrt{P_m}$$

# Two-dimensional systems

## Multi-chain approach

**[S. Liang and H. Pang, Phys. Rev. B. 49, 9214 (1994)]**

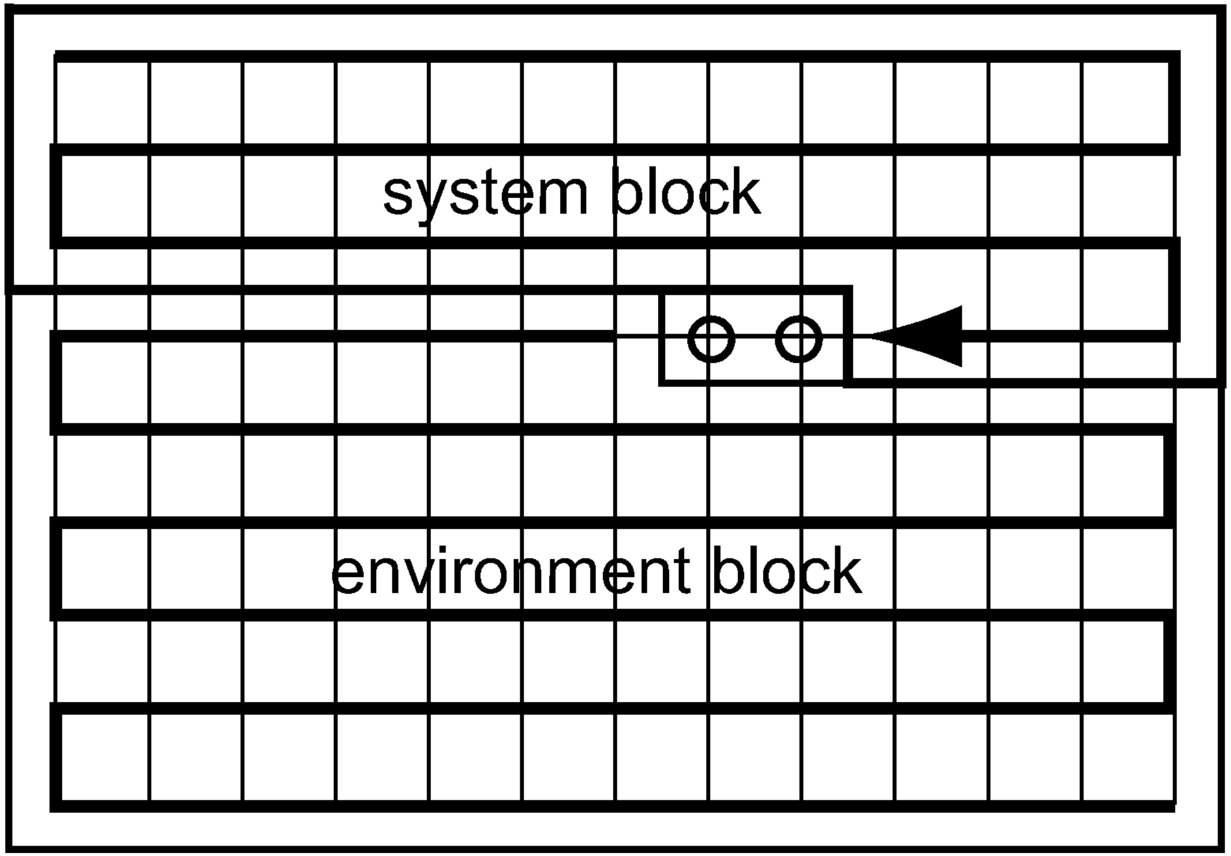



Figure from
U. Schollwöck,
RMP 2005

**Computational cost $\sim$ (chain length)$^{\mathbf{c}}$**
**$\sim$ exp(c$\times$number of chains)**

# Two dimensions vs one dimension

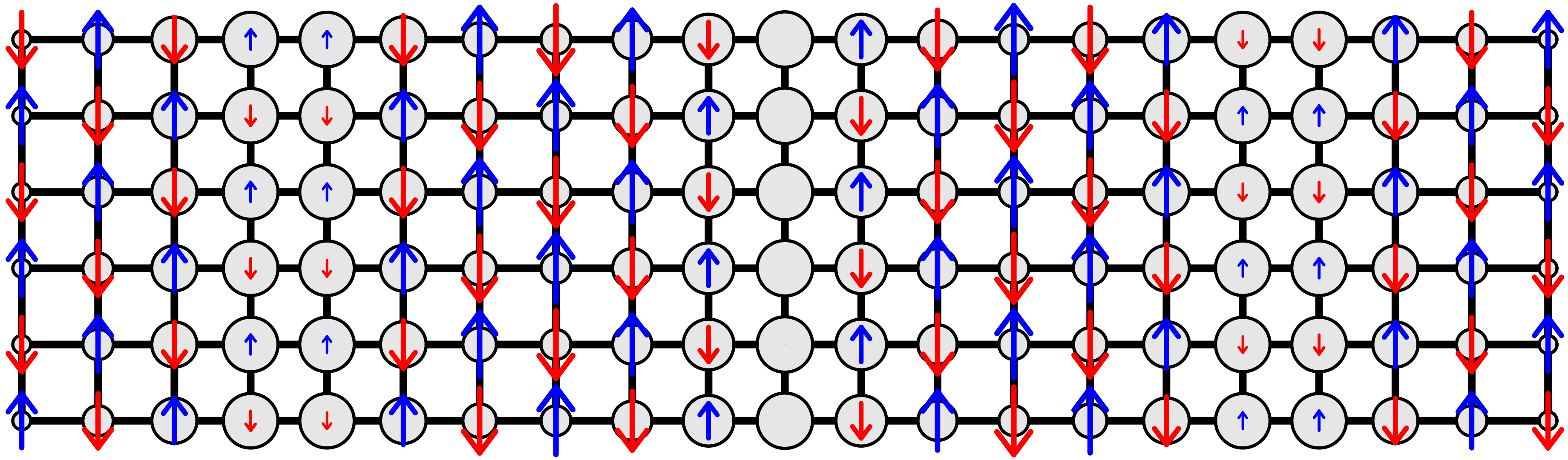
DMRG calculation for the ground state energy of a 16-site Hubbard model at half filling and $U = 12t$

| | open chain | periodic square cluster |
|---|---|---|
| $m$ | 120 | 2400 |
| $P_m$ | $10^{-12}$ | $10^{-6}$ |
| | $\sim 10^{-7} e^{-m/10}$ | $\sim \frac{10^{-2}}{m}$ |
| $\Delta E/t$ | $\approx 10^{-7}$ | $\approx 10^{-3}$ |
| CPU (1999) | 20 seconds | 15 hours |
| Memory | 5 MB | 250 MB |

# Ladder systems

[R. M. Noack, S. R. White, and D. J. Scalapino, Phys. Rev. Lett. 73, 882 (1994)]

**$21 \times 6$ ladder with 12 holes and $U = 12t$**



Among the largest ladder systems studied with DMRG:

- One-band Hubbard model with $(28 \times 6)$ sites
  [G. Hager, G. Wellein, E. Jeckelmann, and H. Fehske, Phys. Rev. B, 2005]

- Three-band Hubbard ladder with $(32 \times 2)$ Cu-sites (and 162 O-sites)
  [S. Nishimoto, E. Jeckelmann, and D.J. Scalapino, Phys. Rev. B, 2002]

# Transfer-matrix renormalization group (TMRG) methods

## Density-matrix renormalization of a transfer matrix

1. **TMRG for classical statistical systems**
   [T. Nishino, J. Phys. Soc. Jpn. **64**, 3598 (1995)]

2. **Corner transfer matrix renormalization group**
   [T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. **65** 891 (1996)]

3. **TMRG for quantum statistical systems**
   [R.J. Bursill, T. Xiang, and G. A. Gehring, J. Phys.: Condens. Matter **8**, L583 (1996); X.Q. Wang and T. Xiang, Phys. Rev. B **56**, 5061 (1997); N. Shibata, J. Phys. Soc. Jpn. **66**, 2221 (1997)]

4. **Quantum TMRG ⇒ Dynamical properties at finite temperature**
   [T. Mutou, N. Shibata, and K. Ueda, Phys. Rev. Lett. **81**, 4939 (1998); (E) **82**, 3727 (1999)]

# Dynamical correlation functions with DMRG

$$\chi_{\hat{A}}(\omega + i\eta) = -\frac{1}{\pi} \langle \psi_0 | \hat{A}^\dagger \frac{1}{E_0 + \omega + i\eta - \hat{H}} \hat{A} | \psi_0 \rangle$$

**Lanczos vector method**

[K. Hallberg, PRB **52**, 9827 (1995)]

$$\begin{aligned} |\phi_0\rangle &= \hat{A}|\psi_0\rangle \\ |\phi_1\rangle &= \hat{H}|\phi_0\rangle - a_0|\phi_0\rangle \\ |\phi_{n+1}\rangle &= \hat{H}|\phi_n\rangle - a_n|\phi_n\rangle - b_n^2|\phi_{n-1}\rangle \end{aligned}$$

$\rho_{\mathrm{L}} = \psi_0\psi_0^* +$ Lanczos vectors

**Correction vector method**

[S. Ramasesha et *al.*, Synth. Met. **85**, 1019 (1997), T.D. Kühner and S.R. White, PRB **60**, 335 (1999)]

$$|CV\rangle = \frac{1}{E_0 + \omega + i\eta - \hat{H}} \hat{A}|\psi_0\rangle$$

$$\chi_{\hat{A}}(\omega + i\eta) = \frac{-1}{\pi} \langle \psi_0 | \hat{A}^\dagger | CV \rangle$$

$\rho_{\mathrm{CV}} = \psi_0\psi_0^* +$ correction vectors

Improved methods: dynamical DMRG and t-DMRG $\rightarrow$ my second talk on Thursday

# DMRG for bosonic systems

Problem: Hilbert space dimension $D = \infty$ for each boson site

Solution: Reduction of the boson Hilbert space with a density-matrix renormalization

1) Pseudo-site method
[E. Jeckelmann and S.R. White, Phys. Rev. B **57**, 6376 (1998)]

2) Optimal basis method
[C. Zhang, E. Jeckelmann, and S.R. White, Phys. Rev. Lett. **80**, 2661 (1998);
A. Weiße, H. Fehske, G. Wellein, and A. R. Bishop Phys. Rev. B **62**, R747 (2000)]

3) Four-block method [R. J. Bursill, Phys. Rev. B **60**, 1643 (1999)]

Recent works:
M. Tezuka, R. Arita, and H. Aoki, Phys. Rev. Lett. **95**, 226401 (2005)
H. Fehske, G. Wellein, G. Hager, A. Weiße, and A. R. Bishop, Phys. Rev. B **69**, 165115 (2004)

Lecture notes: E. Jeckelmann and H. Fehske, cond-mat/0510637

# Non-local systems

1. **Momentum space** (site = Bloch state)
   [S. Nishimoto, E. Jeckelmann, F. Gebhard, and R.M. Noack, Phys. Rev. B **65**, 165114 (2002); T. Xiang, Phys. Rev. B **53**, R10445 (1996)]

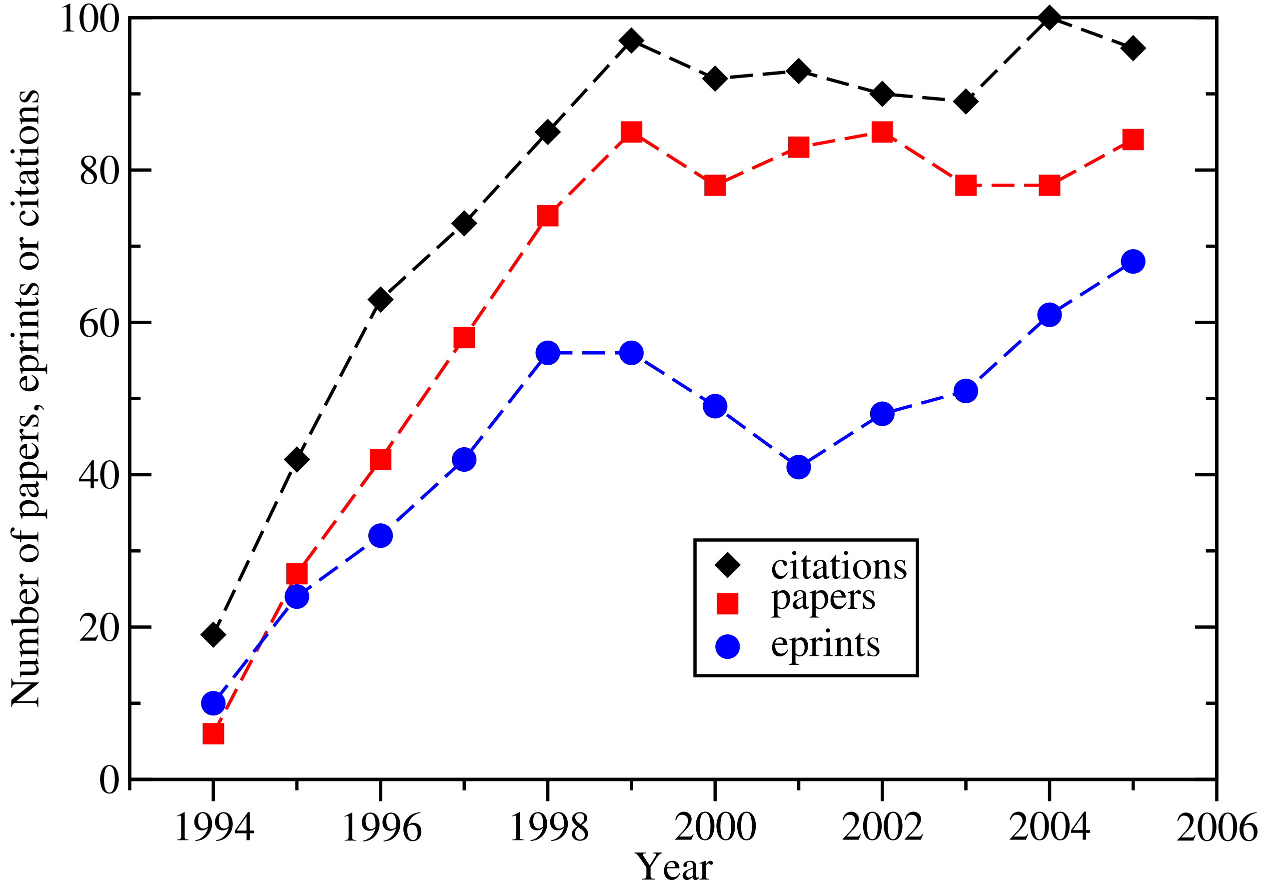
2. **Quantum chemistry** (site = HF or DFT molecular orbital)
   [S. R. White and R. L. Martin, J. Chem. Phys. **110**, 4127 (1999);
   J. Hachmann, W. Cardoen, G.K.-L. Chan, e-print arXiv:cond-mat/0606115]

3. **Nuclear physics** (site = nuclear shell)
   [S. Pittel and N. Sandulescu, Phys. Rev. C **73** 014301 (2006)]

4. **Quantum Hall systems** (site = orbital in a Landau level)
   [N. Shibata and D. Yoshioka, Phys. Rev. Lett. **86**, 5755 (2001);
   J. Phys. Soc. Jpn. **72** 664 (2003) ]

Possible but computationally demanding

# DMRG publications from 1994 to 2005




Annual number of

- published papers on the topic "density[-]matrix renormalization (OR renormalisation)"
- citations to Steve White's original paper [PRL 69, 2863-2866 (1992)], and
- eprints with the string "density matrix renormalization" in their title or abstract.

(a) and (b) from the ISI *Web of Science* database at http://www.isinet.com/, (c) from the *cond-mat* archive of the arXiv e-Print server at http://arxiv.org/.

# More about DMRG

- Book: I. Peschel, X. Wang, M. Kaulke, and K. Hallberg (Eds.), *Density-Matrix Renormalization*, Springer, Berlin, 1999.

- Review article: U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005). E-print: cond-mat/0409292.

- Review article: R.M. Noack and S.R. Manmana, *Diagonalization- and Numerical Renormalization-Group-Based Methods for Interacting Quantum Systems* in AIP Conf. Proc. **789**, 93-163 (2005). E-print: cond-mat/0510321.

- DMRG homepage at http://dmrg.info

- Tomotoshi Nishino's DMRG homepage at http://quattro.phys.sci.kobe-u.ac.jp/dmrg.html

- A DMRG program (C++) for a particle in a box is available on Steve White's homepage at http://hedrock.ps.uci.edu/

- A non-interacting DMRG package (C++) is included in the latest release of the ALPS project (http://alps.comp-phys.org/).

# Summary

- Density-matrix renormalization group (DMRG) method
- Numerical method for correlated systems of spins and fermions
- Highly accurate for static properties of one-dimensional local systems
- Analysis of DMRG truncation errors
- Extensions to finite temperature and 2D classical systems [transfer matrix DMRG (TMRG)] and to bosonic systems
- Extensions to higher dimensions and non-local systems are computationally expensive
- Dynamical properties and time evolution are now possible
  $\Rightarrow$ more in my second talk on Thursday