Implementing the SU(2) Symmetry for the DMRG Algorithm

DMRG++

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Outline

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Symmetries in Diagonalization Methods

- Symmetries block the Hamiltonian, speeding up diagonalization. Most of the time indispensable.
- "Easy symmetries": Think S^z:
  - S^z diagonal in the "natural" Hilbert-space-basis
  - $S^z|a\rangle \otimes |b\rangle = S^z_1|a\rangle \otimes S^z_2|b\rangle$
  - S^z diagonal in product basis, at most need reorder: permutation P
- SU(2) symmetry: Think S^2 (Casimir operator):
  - $S^2|a\rangle \otimes |b\rangle \neq S^2_1|a\rangle \otimes S^2_2|b\rangle$
  - Solution: construct new basis: $G_{c;a+bN_1}|a\rangle \otimes |b\rangle$
  - $G_{c;a+bN_1}$ are more or less Glebsch-Gordan coefficients

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Construction of Basis where S^2 is diagonal

- Problem Consider two orbitals: green and red. How do I construct a state for the new basis? Like this:

$$|c\rangle = |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + \cdots ? \quad (1)$$

- Solution: Only mix states connected by S^+, or S^-, the ladder operators.

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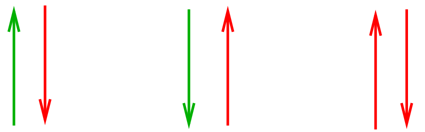

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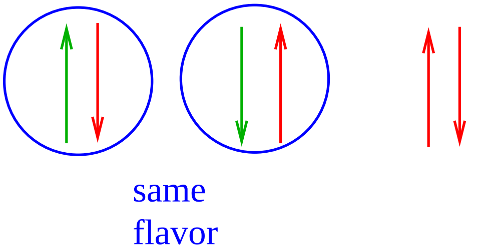

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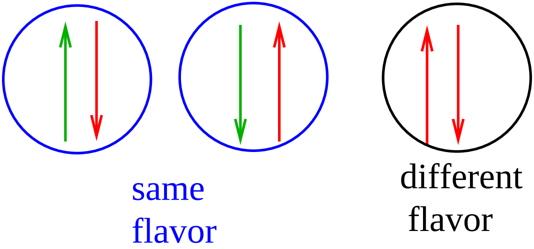

Basis with Full Spin Symmetry

- "Flavor" as equivalence class: $|a_1\rangle \overset{f}{\approx} |a_2\rangle$, if $|a_1\rangle$ and $a_2\rangle$ are connected by S^+: $\exists\, p \in \mathcal{Z}$; $(S^+)^p|a_1\rangle = |a_2\rangle$
- All $|a\rangle$ with the same flavor: (same for $|b\rangle$)

$$|c\rangle = \sum_{a,b} G_{P^{12}(c),a+bN_1} |a\rangle \otimes |b\rangle,$$

- where: $G_{c,a+bN_1} = C^{j_c,j_a,j_b}_{m_c,m_a,m_b} \delta_{f_{a\otimes b},f_c}$.
- "Flavor" of the outer product of states:

$$f_{a\otimes b} \equiv f_a + f_b F_1 + (q_a + q_b Q_1) F_1 F_2 + + (\tilde{j}_a + \tilde{j}_b \tilde{J}_1) F_1 F_2 Q_1 Q_2.$$

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J. F. Cornwell, Group Theory in Physics, Academic Press, London, 1984.

Invariant Density Matrix

- Problem: general density matrix does not preserve m:

$$\rho^{S}_{j_1 m_1 f_1; j'_1 m'_1 f'_1} = \sum_{j_2, m_2, f_2} \psi^{*}_{j_1 m_1 f_1; j_2 m_2 f_2} \psi_{j'_1 m'_1 f'_1; j_2 m2 f_2}. \quad (2)$$

- Solution: we use the invariant density matrix instead: (McCulloch *et al.* Europhys. Lett. 57 (2002) 852.)

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- Speed-up: We use Wigner-Eckart Theorem and Reduced Operators (McCulloch *et al.*)

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M	SU(2) 1 proc	SU(2) 2 procs	Local 1 proc
100	42	41	67
200	160	136	319
300	335	290	808
400	544	485	1602
800	3020	2526	$>$2 hours

Table: Times in seconds to run the one-orbital Hubbard model on 32 sites at half filling, with $U = t = 1$. Runs done with 2 processors used shared memory parallelization with *pthreads*.

Parallelization with *Pthreads*: Overview

- CPU intensive part: sum over connections of form $c_i^\dagger c_j$ (Hubbard), $S_i^+ S_j^-$, $S_i^z S_j^z$ (Heisenberg), and generally:

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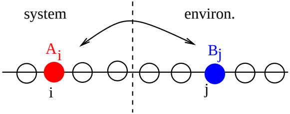

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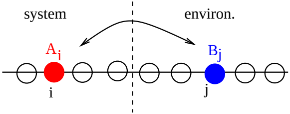

- The sum over i, j

$$\sum_{\text{connections}\, i,j} A_i B_j \tag{4}$$

can be parallelized efficiently using *pthreads*.

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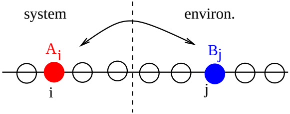
$$(A^S B^E)_{c,c'} = \sum_{a,b,a',b'} G^{SE}_{P^{SE}(c),a+bN_s} \left(\tilde{s}_a A^S_{a,a'} B^E_{b,b'}\right) \times G^{SE}_{P^{SE}(c'),a'+b'N_s}$$



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Parallelization In Action: A Model For The Pnictides

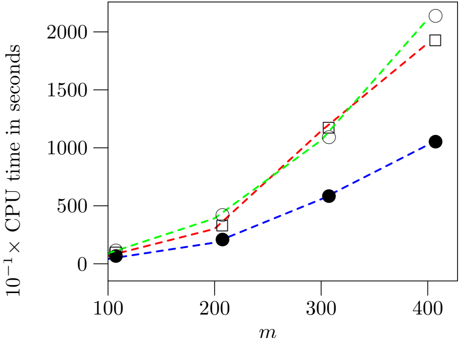

Figure: Serial (red/green lines) vs. Parallel (blue lines)

Our work on DMRG for pnictides is here:
Phys. Rev B. **81** 085106 (2010)

DMRG++: A generic DMRG Code

- User Interface: can be used without need to understand the code
- Code is generic: any model, any geometry, easy to extend
- Performance is taken into account but not the main goal.
- Considers symmetries, and parallelization when possible

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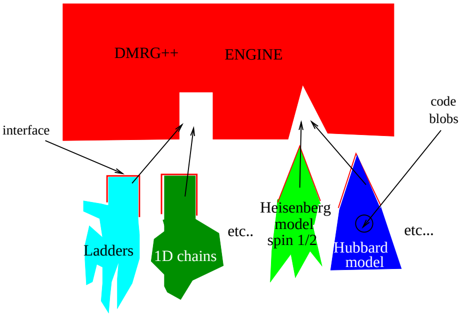
DMRG++ Generic Interfaces



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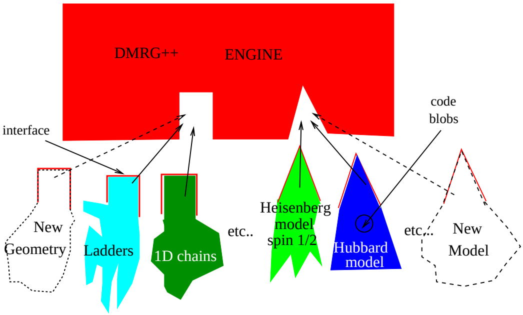
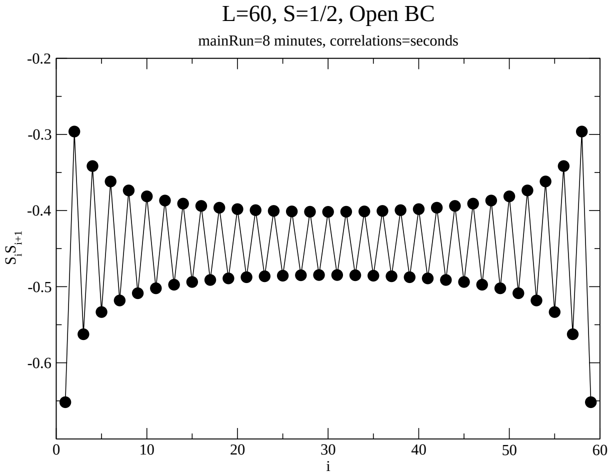


Observables: Back to the '90s



Compare to: Fig 6(a) of S. White, Phys. Rev. B 48, 10345, (1993)

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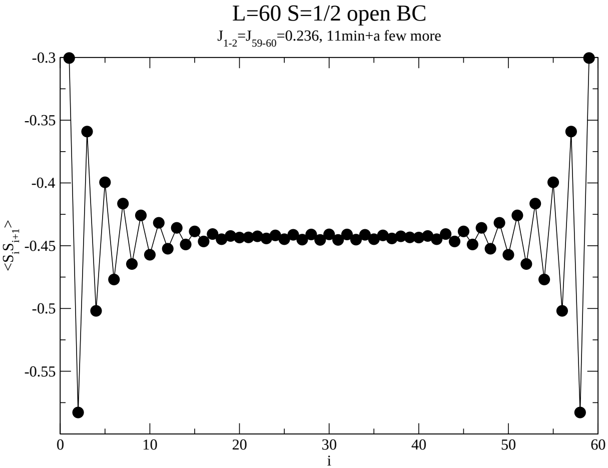

Compare to:Fig 6(c) of S. White, Phys. Rev. B 48, 10345, (1993)

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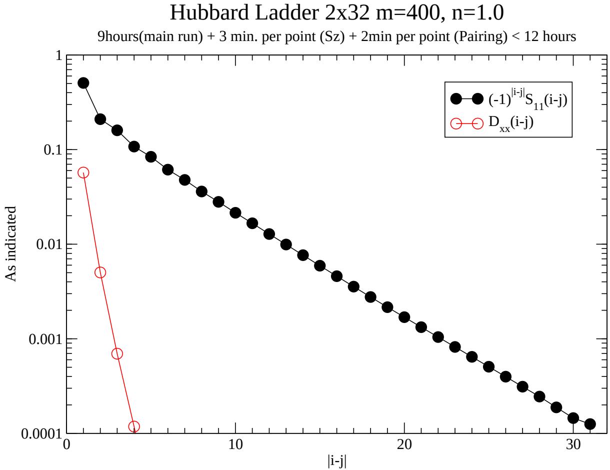

Compare to: Fig 3 of Noak, White, Scalapino, `http://arxiv.org/abs/cond-mat/9404100v1` (1994)

Partial TODO List: There's lot more to do!

- Other models (e.g. t-j model)
- Other geometries (e.g. “trees”)
- WaveFunctionTransformation: Needs to run faster
- Engine: Performance needs to improve
- Concurrency:
  More agressive parallelization

[Wikimedia Commons]

Summary

- SU(2) Symmetry accelerates the DMRG algorithm.
- Shared memory parallelization useful when having many Hamiltonian connections $A_i B_j$.
- DMRG++ codebase implements all this generically.

Thanks to: E. Dagotto, L. G. G. V. Dias da Silva, I.P. McCulloch, J. A. Riera, T. C. Schulthess, M.S. Summers.

- http://arxiv.org/abs/1003.1919
- http://arxiv.org/abs/0902.3185 published in CPC.
- http://www.ornl.gov/~gz1/dmrgPlusPlus/

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Credit Line

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