•The J-DMRG and the Nuclear Shell Model

- Will describe current status of a program to develop an angular-momentum-conserving variant of the Density Matrix Renormalization Group method (the J-DMRG) for use in approximate large-scale shell model calculations.
- Recent work carried out primarily with my former graduate student, *Bhupender Thakur,* now at the LONI Institute and Center for Computational Technology at LSU.
- Early results of our work reported in:

  B. Thakur, SP and N. Sandulescu, Phys. Rev. **C**78 (2008) 041303.
- More recent results and the general formalism reported in

  Bhupender Thakur, Ph.D. thesis, University of Delaware, 2010, unpublished.

  Stuart Pittel and Bhupender Thakur, Acta Physica Polonica **B** 42 (2011)427.

Outline of Talk

- Overview of the DMRG method and how we apply it to atomic nuclei
- Results of systematic calculations for nuclei in the *1f-2p* shell
- Summary and future outlook

Overview of the DMRG

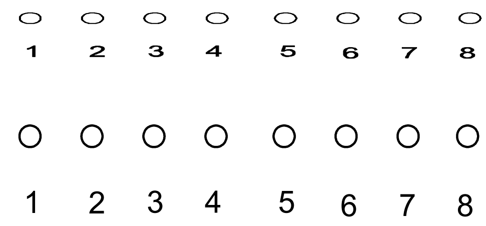
- The Density Matrix Renormalization Group (DMRG) was first introduced by Steven White in early 90s to treat properties of quantum lattices, where it was extremely successful.
- Original formulation based on iterative inclusion of real-space lattice sites.
- Subsequently reformulated to iteratively add momentum or energy levels, rather than real-space lattice sites. Reformulated version has proven useful in describing several finite Fermi systems (quantum chemistry; small metallic grains; 2D electron systems).
- Suggests possible use in description of another finite Fermi system, the atomic nucleus.
- Review article: J. Dukelsky and SP, Rep. Prog. Phys. 67 (2004) 513.

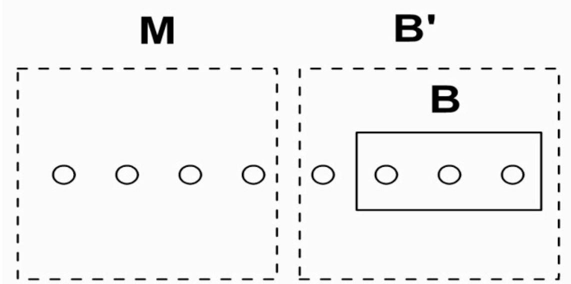
DMRG Growth Procedure and Truncation Strategy

- *Sites:* Begin with introduction of an ordered set of 'sites', which in nuclear shell model represent single-particle orbitals. Will assume they are spherical.

- *Enlargement:* Starting with a *block* **B** representing a set of sites (and containing *m* states) , enlarge to include the next site, thereby producing an *enlarged block* **B'**.

- *The Medium:* The rest of the sites comprise the *medium* **M**.





DMRG Growth Procedure

- *Truncation:*
  - Couple enlarged block to medium and diagonalize resulting *superblock* hamiltonian. Ground state (g.s.) written as

$$|\psi_{GS}> = \sum_{i \subset B'} \sum_{j \subset M} \psi_{ij} \, |i>_{B'} \, |j>_{M}$$

  - Reduced density matrix of enlarged block in g.s. is constructed, then diagonalized:

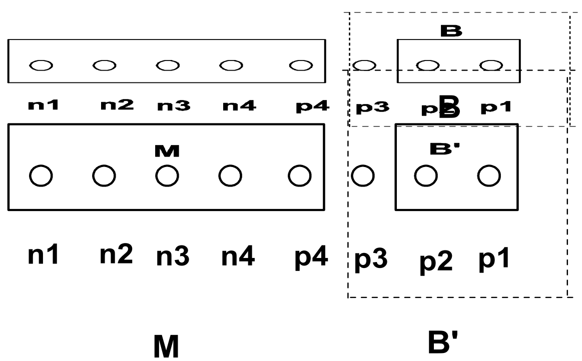
$$\rho_{ii'}^{B'} = \sum_{j \subset M} \psi_{ij}^{*} \psi_{i'j}$$

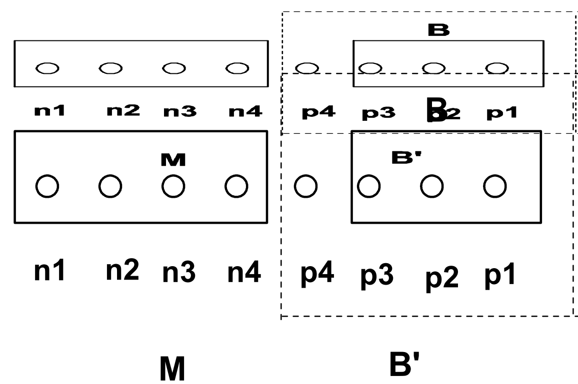
  - Truncate to *m* eigenstates with the largest eigenvalues, *same number as before enlargement. Guaranteed* to be the *m most important* states of enlarged block in ground state of superblock.
  - Can treat mixed density matrices, whereby info from several states of interest is included.
- *Renormalization:* Renormalize all operators from enlarged block to act in this *optimum* truncated space.

A Typical DMRG Calculation – with nuclei in mind

- *Warmup Phase:* Make initial guess on the optimal states (for a given *m*) of each block. The better the guess the more rapid the convergence of the iterative process.

- *Sweep phase:* Gradually sweep thru sites, using for the medium the results either from the warmup phase or from the previous sweep.

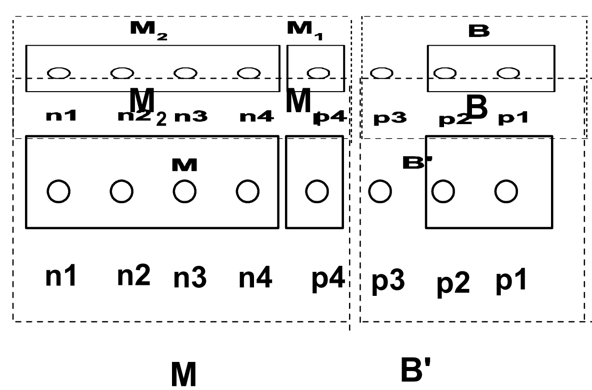




- *Iteration:* Sweep thru the sites over and over until convergence from one sweep to the next is achieved.

- *Convergence with m:* Do the calculations as a function of the number of retained states *m* until changes are acceptably small.

- In our calculations, we use a three-block growth strategy:
  - We always have neutron and proton orbits on opposite ends of the chain.
  - We do not build mixed blocks.
  - In the sweep stage, we go to and from through the orbits of a given type of particle only.
  - The full medium **M** typically involves two components, $\mathbf{M_1}$ and $\mathbf{M_2}$.



Key Calculational Constructs

- At each growth or enlargement step, must evaluate matrix elements of all hamiltonian sub-operators,

$$a_i^+,\ a_i^+ a_j,\ a_i^+ a_j^+,\ a_i^+ a_j^+ a_k,\ a_i^+ a_j^+ a_k a_l\ ,\ +\ h.c.,$$

and store them.

- Having this info for block and additional level makes it possible to calculate it for enlarged block.

- Having it for medium also makes it possible to calculate superblock hamiltonian.

J-DMRG

- In most applications of DMRG, states are constructed as direct products of states from each block. In nuclei, this means working in m-scheme. Because of truncation, this typically leads to loss of good angular momentum and thus to loss of some correlations.

- Thus, we use an angular-momentum-conserving variant of the method (called the J-DMRG), whereby we couple angular momentum eigenstates of each block.

- Main difference with regards to ordinary DMRG is that we need to calculate and store *reduced matrix elements* of all hamiltonian sub-operators at each stage.

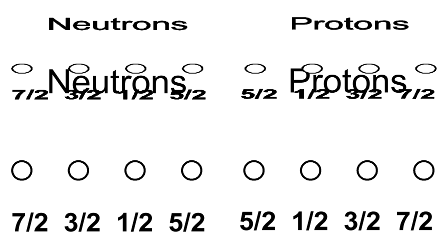
- J-DMRG also applied to nuclei in context of Gamow Shell Model , see e.g. J. Rotureau, N. Michel, W. Nazarewicz, M. Ploszajczak and J. Dukelsky, Phys.Rev. C79, 014304 (2009) .

Results

- Will report results for shell model calculations of nuclei from ^{48}Cr to ^{56}Ni. In all cases we assume an inert ^{40}Ca core and distribute the remaining particles over the levels of the *2p-1f* shell.

- In all calculations, we use GXPF1A hamiltonian, which provides good description of nuclei in this region. We compare our results with those of exact SM calculations (where available) to assess the method.

- We use the following order of single-particle orbitals in the *chain*:



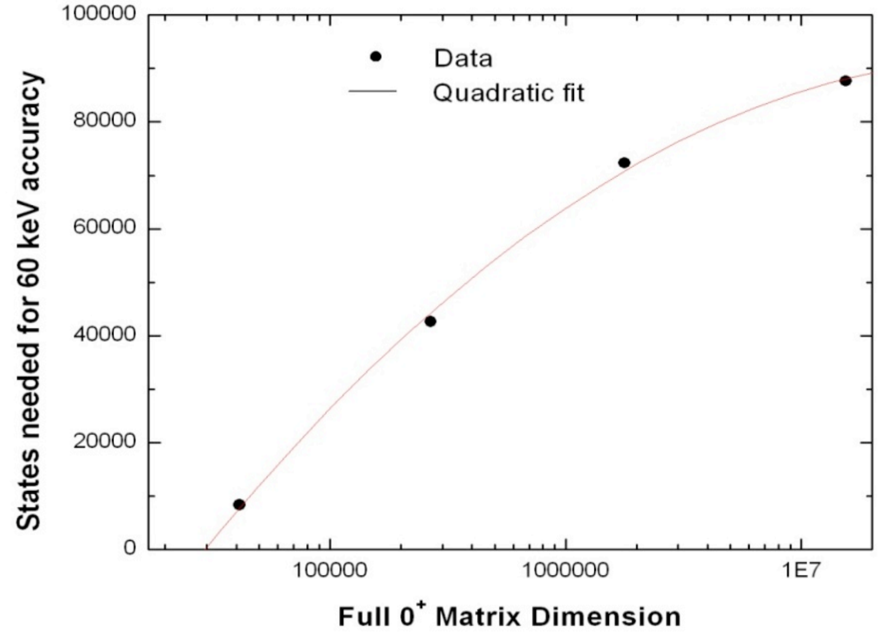
Ground states of even-even nuclei

Have studied ^{48}Cr, ^{50}Cr, ^{52}Fe, ^{54}Fe and ^{56}Ni. In all cases, the results converge smoothly with *m* to the exact ground state energy.

m	E_{GS} (MeV)	Max Dim
100	-205.643	87,633
120	-205.651	106.383
140	-205.652	123,196
160	-205.659	139,166
180	-205.661	166,695
200	-205.670	199,274
Exact	-205.709	15,443,684

^{56}Ni

Scalability of the Method for even-even nuclei



By extrapolating fit we conclude that we can use method to describe nuclei with well in excess of 10^9 0^+ configurations to within 60 keV accuracy, using matrices of at most a few hundred thousand states.

Ground states of odd-mass nuclei

Have studied ^{47}Cr, ^{49}Cr, ^{51}Fe, ^{53}Fe and ^{55}Ni. Here, too, the results systematically converge with *m* to the exact results. For larger nuclei , however, cannot do better than about 90 *keV* accuracy, because the spaces get too large for us to carry out diagonalizations for larger *m*.

m	**E_{GS} (MeV)**	**Max Dim**
50	-189.412	450,916
70	-189.426	529,911
90	-189.435	663,686
Exact	-189.534	63,268,915

^{55}Ni

For odd-mass nuclei, fraction of space required for good accuracy likewise goes down rapidly with size of problem, but not as strikingly as for e-e nuclei.

Excited states

- Once an optimal block structure determined, even if from properties of g.s. only, can use it to estimate excited states. Simply couple optimal blocks to the appropriate angular momentum and diagonalize *H*.

m	$E_{0_1^+}$ (MeV)	$E_{0_2^+}$ (MeV)
140	-205.652	-200.913
160	-205.659	-200.902
Exact	-205.709	-202.092

← *g.s. and 1st excited 0+ state in ^{56}Ni: Targeting g.s only.*

g.s. and 1st excited 0+ state in ^{56}Ni: Targeting both states. →

m	$E_{0_1^+}$ (MeV)	$E_{0_2^+}$ (MeV)
140	-205.641	-201.739
160	-205.645	-201.752
Exact	-205.709	-202.092

Excited states: odd-mass nuclei

- Here too can target just g.s. or several low-lying states. Easier to target several low-lying states in odd-mass nuclei than in even-even nuclei, because of dimensionality considerations. In e-e nuclei, non-0^+ states have very different dimensionalities than 0^+ states. In odd-mass nuclei, all relevant J^π values typically have similar dimensions .

Calculated results for ^{53}Fe in *MeV*

m	**$7/2_1^-$**	**$3/2_1^-$**
50	-162.528	-161.546
60	-162.530	-161.606

Target $7/2_1^-$ only

$7/2_1^-$	**$3/2_1^-$**	***m***
-162.484	-161.735	50
-162.528	-161.743	60

Target both $7/2_1^-$ and $3/2_1^-$

Outlook for the future

- J-DMRG method seems to converge and scale very well and seems capable of describing all low-lying states with acceptable accuracy.

- Key current limitation is our ability to carry out in an appropriately timely fashion the larger diagonalizations (often over and over) that will arise in larger calculations. Especially true with the larger single-particle orbitals that arise in heavier nuclei. Thus, we urgently need an improved diagonalization algorithm.

-Assuming we are able to overcome this bottleneck, we should be in a position to carry out a wide range of large-scale shell-model calculations of nuclei not currently amenable to exact treatment. Can also include other observables not discussed here.

- *Applications*: First applications we anticipate will be to nuclei in the mass-80 region, including the $g_{9/2}$ orbital. Issues related to spurious center-of-mass motion effects currently under investigation.