UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional

San Diego State University

Configuration-Interaction Calculations of the Unitary Fermi Gas: Convergence, Densities, and all that

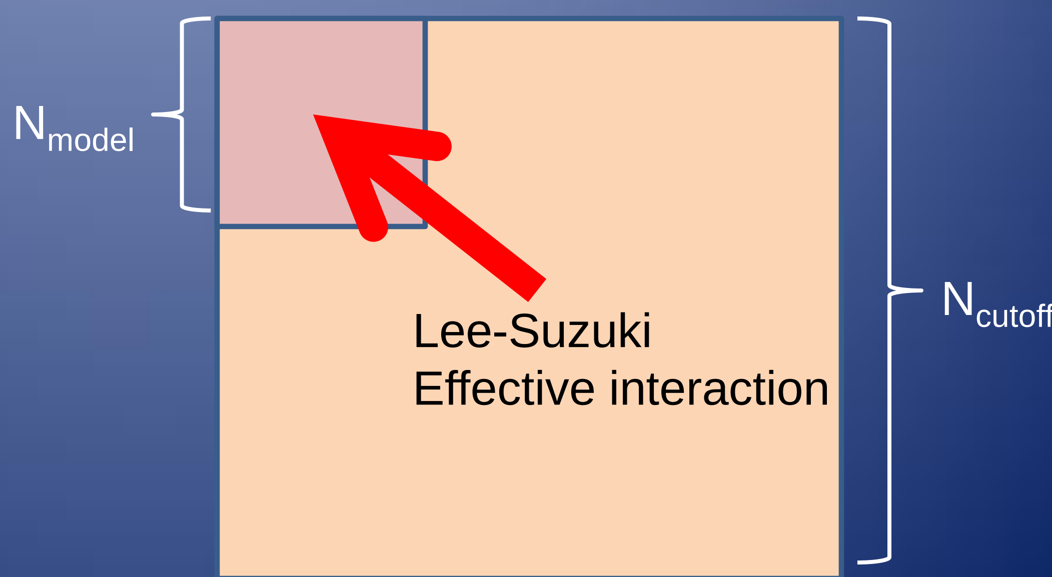
Calvin Johnson, San Diego State University
Hai Ah Nam, SDSU
Erich Ormand, Lawrence Livermore
+ Alhassid, Bertsch, Fang, Fujii….

CI: Diagonalize Hamiltonian in a basis of Slater determinants with h.o. single-particle states

The "Bertsch Problem": Cold gas of atoms with infinite scattering length in an external harmonic trap

Proposed test bed for many-body methods; non-perturbative

Truncation in relative frame



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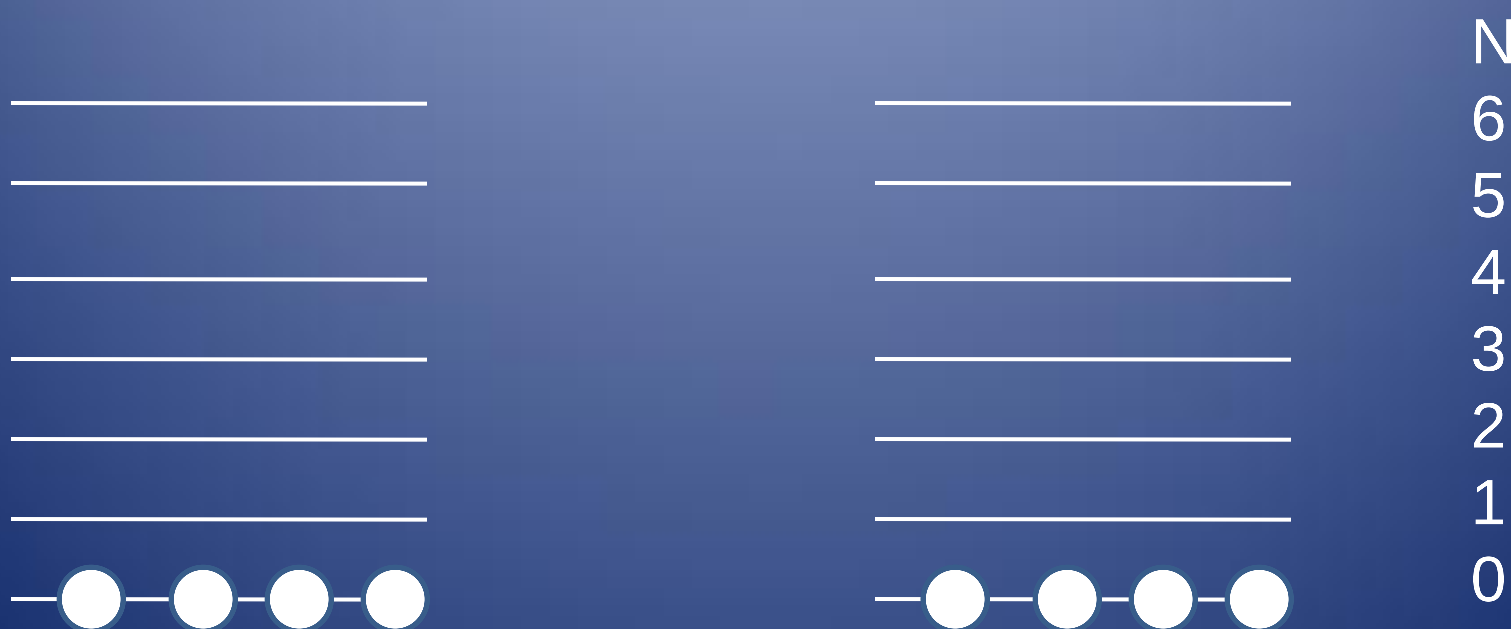
Two kinds of truncations in lab frame

"Orbital truncation"
All particles can be excited up to N_{max} orbit

"Energy truncation"
Truncated based upon summed N_{excite} energy



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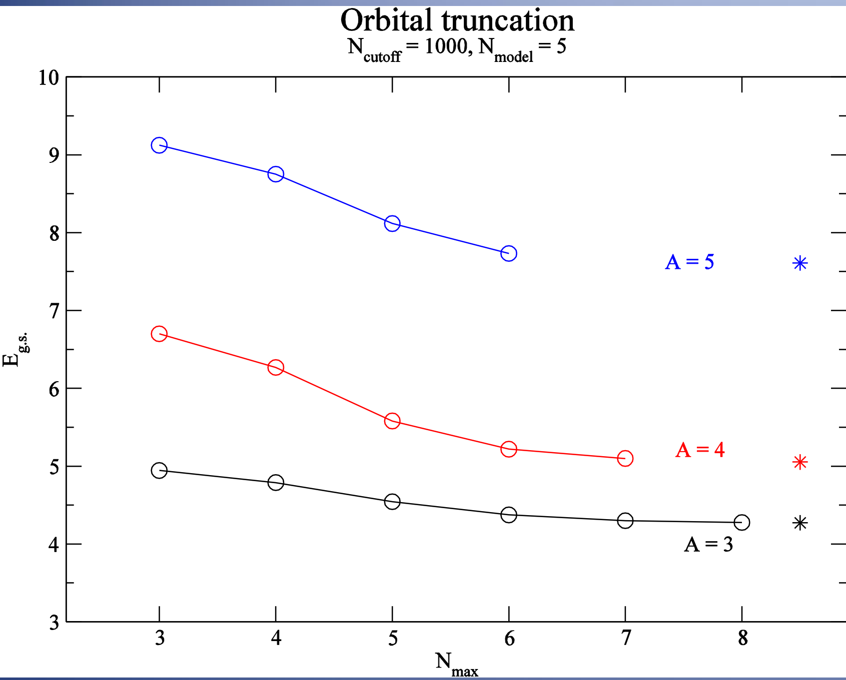
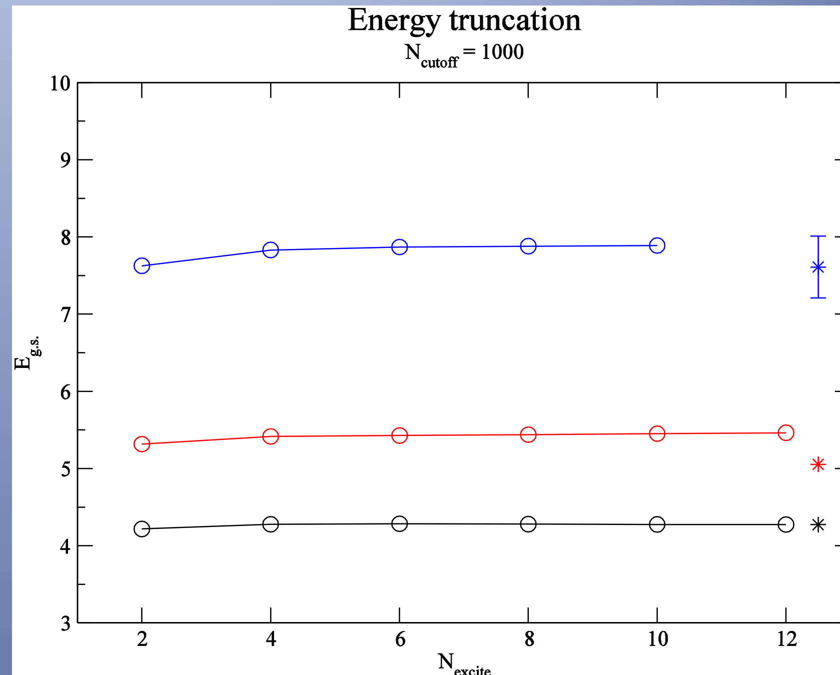
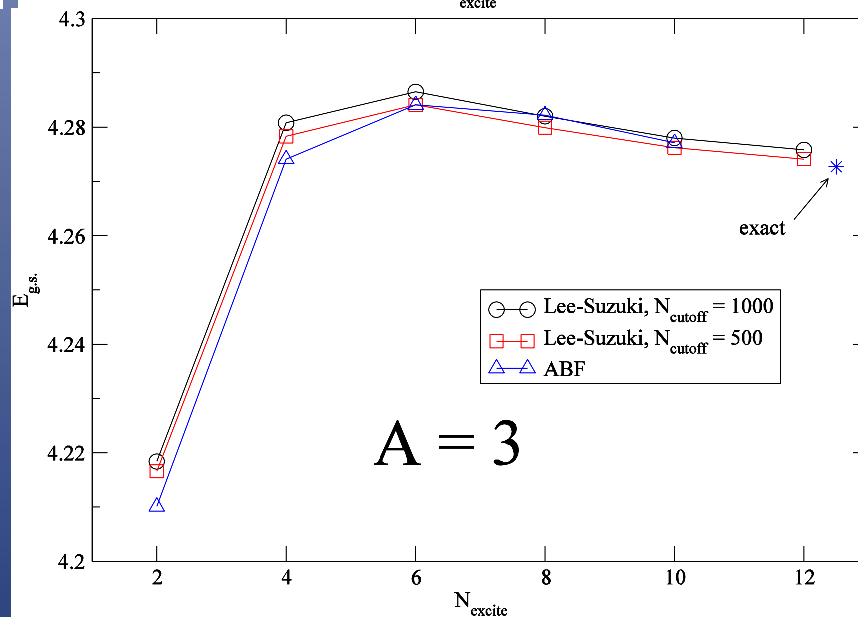
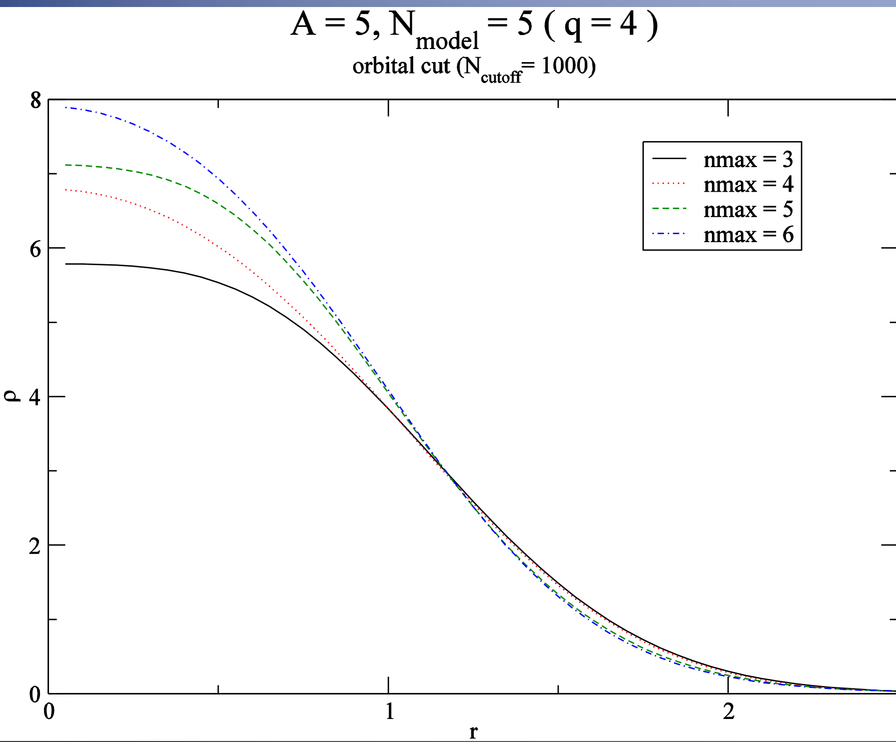
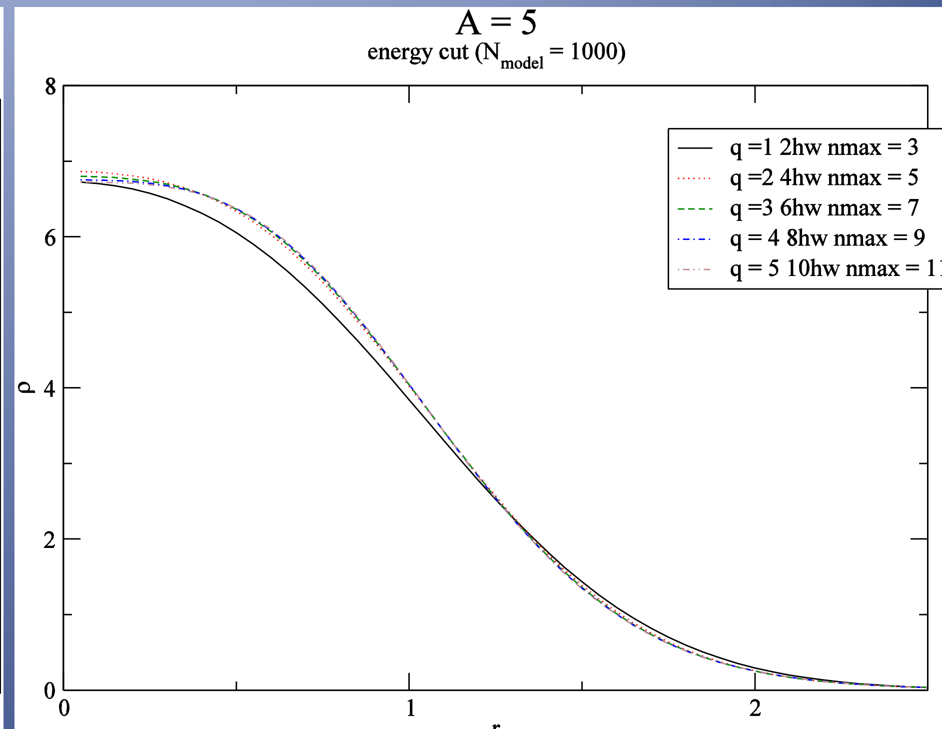






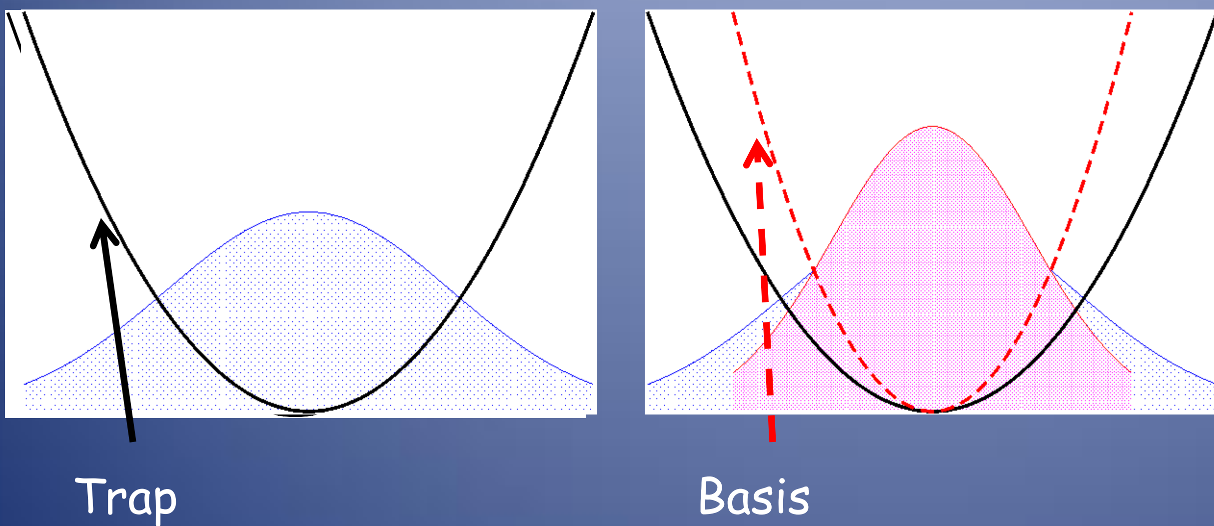
Density profiles
computed from 1-body density matrices





NB: discrepancy not as bad for A = 3

Scale of "naïve" basis defined by external trap incommensurate with mean field….



In any h.o. basis, we can define a (nondiagonal) harmonic trap with *hw* = 1 by

$$\frac{1}{2}\left(\frac{1}{B^2}\hat{P}^2 + B^2\hat{X}^2\right)$$

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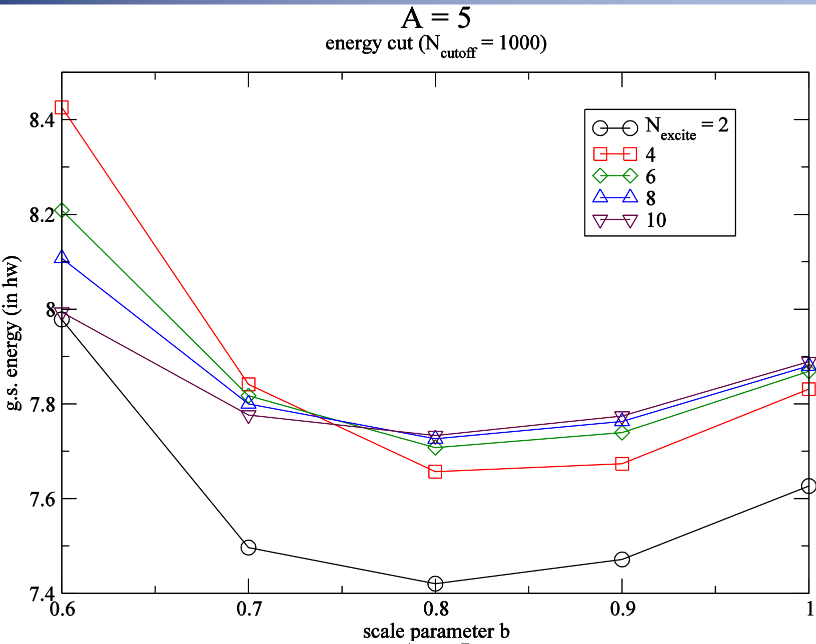
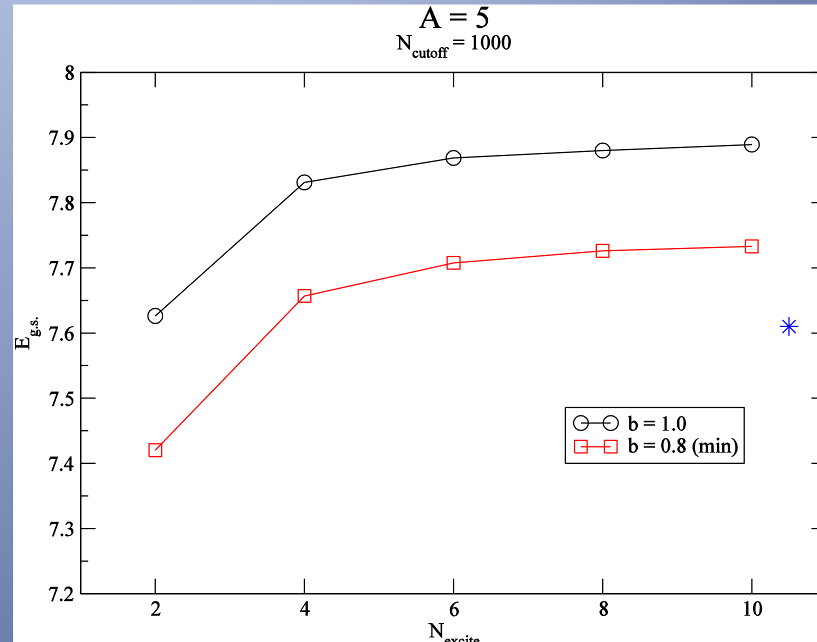
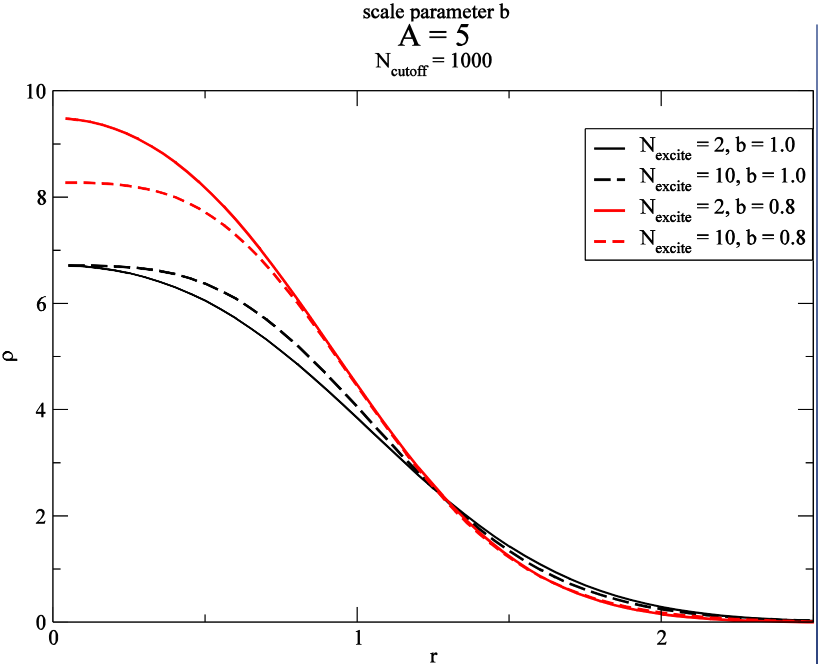
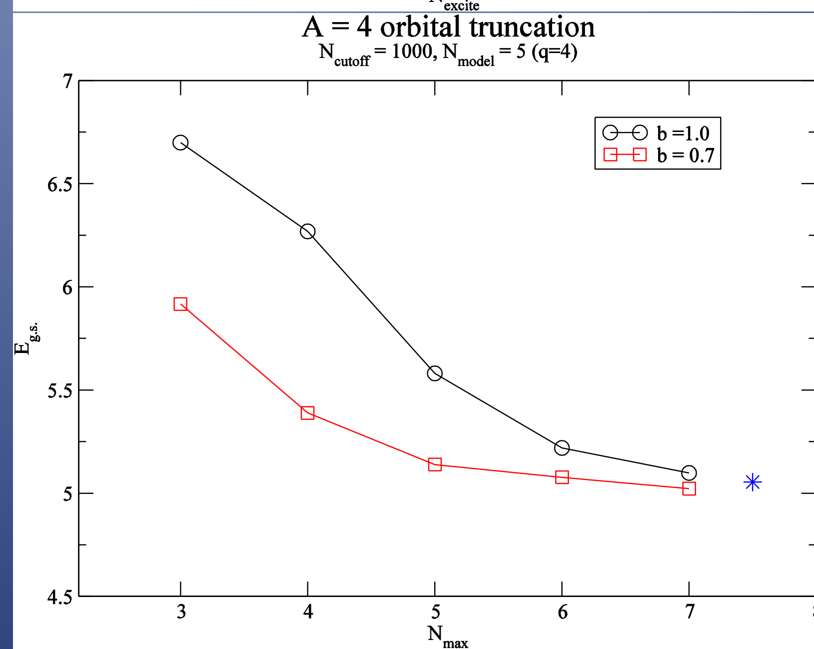








REDSTICK : CI-solver with 3-body forces

(With 2-body forces can do 400-500M states on single processor)

H. Nam improved efficiency of application of 3-body Hamiltonian in REDSTICK

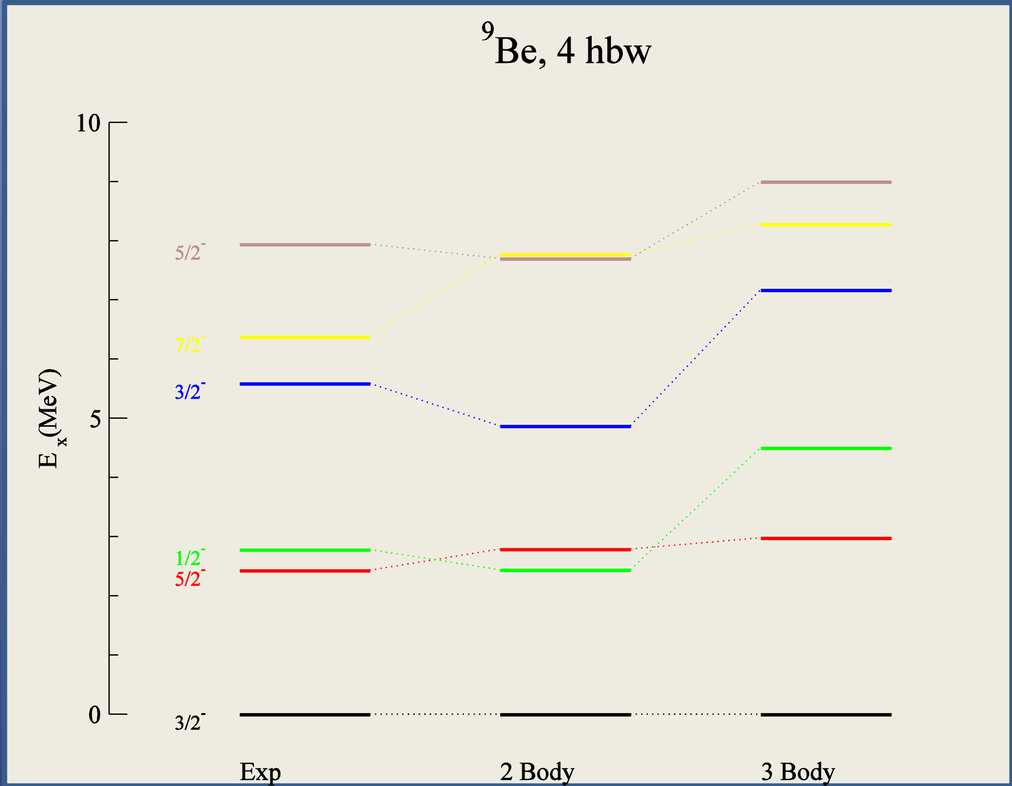
* speed-up by factor 3-4
* makes calculations with 5-50M basis states practical
* Now load-balance limited

This summer :

* Gamow-Teller transition in ^{9}Be at 4, 6hw
* Effective single-particle spectrum in ^{15,17}O

G.S. binding energy (4hw)

Exp	-58.16
2Body	-54.80
3Body	-59.82



Work Plan Year 2.5 (rest of 2008)

*UNEDF-funded postdoc – Plamen Krastev – starts next week.
* Continue convergence study for UFG
  ** Determine whether UFG a good model for the nucleus.
   → Look at finite-range, ∞-scatt length gas (+JS) .

* Detailed study of incommensurate basis for UFG
* Study incommensurate basis for nucleus

* Generalize REDSTICK density matrix routines to stand-alone
* Generalize density matrix routines to spectroscopic factors

JS = Joshua Staker, Physics MS student

Work Plan Year 2.5-3.0 (2008/9)

Improvements to REDSTICK (P. Krastev, new postdoc)
* Improve load-balance for both 2-body / 3-body routines
* Distribute 3-body input data (~3-20 GB) across nodes

** Requirements for 8hw ^{9}Be, 6hw ^{12}C w/3-body interaction
"only" 50M basis states.. But….
Many-body Hamiltonian has about 10^{12} nonzero m.e.s
= ~ 5-20 TB storage (if one uses MFD code) or ~5-10,000 cores
Our on-the-fly code should do this on ~500-1,000 cores

Work Plan Year 3

* Mean-field basis for Lee-Suzuki transformation for nucleus
(in collaboration with Livermore)

THE BIG GOAL:
Push 3-body by another factor of 10:
500M basis states: = 10hw ^{9}Be, 8hw ^{12}C
requires about 50x as much memory
This is truly a challenging computational problem!

* Further improve distribution of "jumps" (decomposition of the action of the Hamiltonian)
-- detailed load-balancing
* Improved diagonalization: "thick-restart" Lanczos, PARPACK, etc.

Team REDSTICK

Erich Ormand, Livermore
Calvin Johnson, SDSU

Hai Ah Nam, SDSU (PhD student, Computational Science)
Supported by Fellowship from Livermore

Plamen Krastev, SDSU (new UNEDF-funded postdoc)*

Joshua Staker, SDSU (MS student, supported on DOE grant)

*first time UNEDF funded personnel will work on this project