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

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Hai Ah Nam, SDSU
Erich Ormand, Lawrence Livermore
+ Alhassid, Bertsch, Fang, Fujii….

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

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

Truncation in relative frame

Lee-Suzuki Effective interaction

N_{\text{cutoff}}

N_{\text{model}}
Two kinds of truncations in lab frame

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<tr>
<th>&quot;Orbital truncation&quot;</th>
<th>&quot;Energy truncation&quot;</th>
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<tr>
<td>All particles can be excited up to $N_{\text{max}}$ orbit</td>
<td>Truncated based upon summed $N_{\text{excite}}$ energy</td>
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<tr>
<th>$N$</th>
<th>6</th>
<th>5</th>
<th>4</th>
<th>3</th>
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Density profiles computed from 1-body density matrices

**A = 5, N_{model} = 5 (q = 4)**

orbital cut ($N_{cutoff} = 1000$)

**A = 5**

energy cut ($N_{model} = 1000$)

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 $\hbar\omega = 1$ by

$$\frac{1}{2}\left(\frac{1}{B^2}\hat{P}^2 + B\hat{X}^2\right)$$
**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 $^9\text{Be}$ at 4, 6hw
* Effective single-particle spectrum in $^{15,17}\text{O}$

**G.S. binding energy (4hw)**

- Exp: -58.16
- 2Body: -54.80
- 3Body: -59.82

![Graph showing energy levels for $^9\text{Be}$ at 4 hw]
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, $\infty$-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