Green's function Monte Carlo Calculations of Light Nuclei

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Work not possible without

NERSC IBM SP (Seaborg)

(421K CPU-hours ≈ 150 TFLOP hours in FY02)

Argonne Math. & Comp. Science Division (Chiba City)

(Est. 900K CPU-hours ≈ 110 TFLOP hours in FY02)

Argonne Laboratory Computing Resource Center (Jazz)

(170K CPU-hours ≈ 95 TFLOP hours since Nov 2002)

Two Problems in Microscopic Few- & Many-Nucleon Calculations

(I) What is the Hamiltonian?

- NN force is reasonably controlled
- 3N force must be determined while computing properties of light nuclei!

(II) Given $\mathcal{H}$, solve the Schrödinger equation for A nucleons accurately.

- Much recent progress for $A \leq 12$

Direct comparison of calculations to data is ambiguous if (II) is not solved.

Our goal is a microscopic description of nuclear structure and reactions from bare NN & 3N forces and consistent currents.

Nuclear Hamiltonian

$$\mathcal{H} = \sum_i K_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

v_{ij}: Argonne v_{18}

$v_{ij} = v_{ij}^{\gamma} + v_{ij}^{CI} + v_{ij}^{CD}; \qquad v_{ij}^{CI} = \sum_{p=1,14} v_p(r_{ij}) O_{ij}^{p}$
$O_{ij}^{p=1,14} =$
$[1, \sigma_i \cdot \sigma_j, S_{ij}, \mathbf{L} \cdot \mathbf{S}, \mathbf{L}^2, \mathbf{L}^2 \sigma_i \cdot \sigma_j, (\mathbf{L} \cdot \mathbf{S})^2] \otimes [1, \tau_i \cdot \tau_j]$

V_{ijk}: Urbana IX and new Illinois models

Need to solve

$$\mathcal{H}\Psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_A; s_1, s_2, \cdots, s_a; t_1, t_2, \cdots, t_A)$$
$$= E\Psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_A; s_1, s_2, \cdots, s_a; t_1, t_2, \cdots, t_A)$$

s_i are nucleon spins: $\pm\frac{1}{2}$
t_i are nucleon isospins (proton or neutron): $\pm\frac{1}{2}$
$2^A \times \binom{A}{Z}$ complex coupled 2^{nd} order equations in $3A - 3$ variables
(number of isospin states can be reduced)

^{12}C: 270,336 coupled equations in 33 variables

Variational Monte Carlo

Minimize expectation value of $\mathcal{H}$

$$E_T = \frac{\langle \Psi_T | \mathcal{H} | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0$$

Simplified trial wave function:

$$|\Psi_T\rangle = [1 + \sum_{i<j<k} U_{ijk}][\mathcal{S} \prod_{i<j} (1 + U_{ij})] \prod_{i<j} f_{ij} |\Phi\rangle$$

U_{ijk} are 3-body correlations from V_{ijk}
U_{ij} are non-commuting 2-body correlations from v_{ij}
f_{ij} are central (mostly short-ranged repulsion) correlations

Φ is a $1\hbar\omega$ shell-model w.f.

- determines quantum numbers of state
- fully antisymmetric
- translationally invariant
- has multiple spatial-symmetry components

Green's Function (Diffusion) Monte Carlo

VMC Ψ_T propagated to imaginary time τ:

$$\begin{aligned} \Psi(\tau) &= e^{-(\mathcal{H}-E_0)\tau}\Psi_T \\ \Psi_0 &= \lim_{\tau\to\infty}\Psi(\tau) \\ \mathcal{H}\Psi_0 &= E_0\Psi_0 \end{aligned}$$

Small time-step propagator:

$$\Psi(\tau) = \left[e^{-(\mathcal{H}-E_0)\triangle\tau}\right]^n \Psi_T; \quad \tau = n\triangle\tau$$

$$G_{\beta\alpha}(\mathbf{R}',\mathbf{R}) = \langle \mathbf{R}',\beta| e^{-(\mathcal{H}-E_0)\triangle\tau} |\mathbf{R},\alpha\rangle$$

$\Psi(\mathbf{R}_n,\tau) =$
$\int G(\mathbf{R}_n,\mathbf{R}_{n-1})\cdots G(\mathbf{R}_1,\mathbf{R}_0)\Psi_T(\mathbf{R}_0)d\mathbf{R}_{n-1}\cdots d\mathbf{R}_0$

^{12}C: 400 steps means 14,000-dimensional integral

Fermion sign problem limits maximum τ:
G brings in lower-energy boson solution
$\langle\Psi_T|\mathcal{H}|\Psi(\tau)\rangle$ projects back fermion solution
Exponentially growing statistical errors

Constrained-path propagation removes steps that have

$$\overline{\Psi(\tau,\mathbf{R})^\dagger\Psi(\mathbf{R})} = 0$$

Many tests demonstrate reliability

Making It Parallel

Master-slave structure

Each slave gets configurations to propagate

Results sent back to master for averaging as generated

During propagation, configs multiply or are killed

- Work load fluctuates
- Periodically master collects statistics and tells slaves to redistribute
- Slaves have work set aside to do during this synchronization
- Would be nice to have MPI construct for this

Large calculations have very low (minutes) frequency of communication

Parallelization efficiencies typically 95%

92% efficency obtained on 2048-processor Seaborg run; 0.55 TFLOPS.

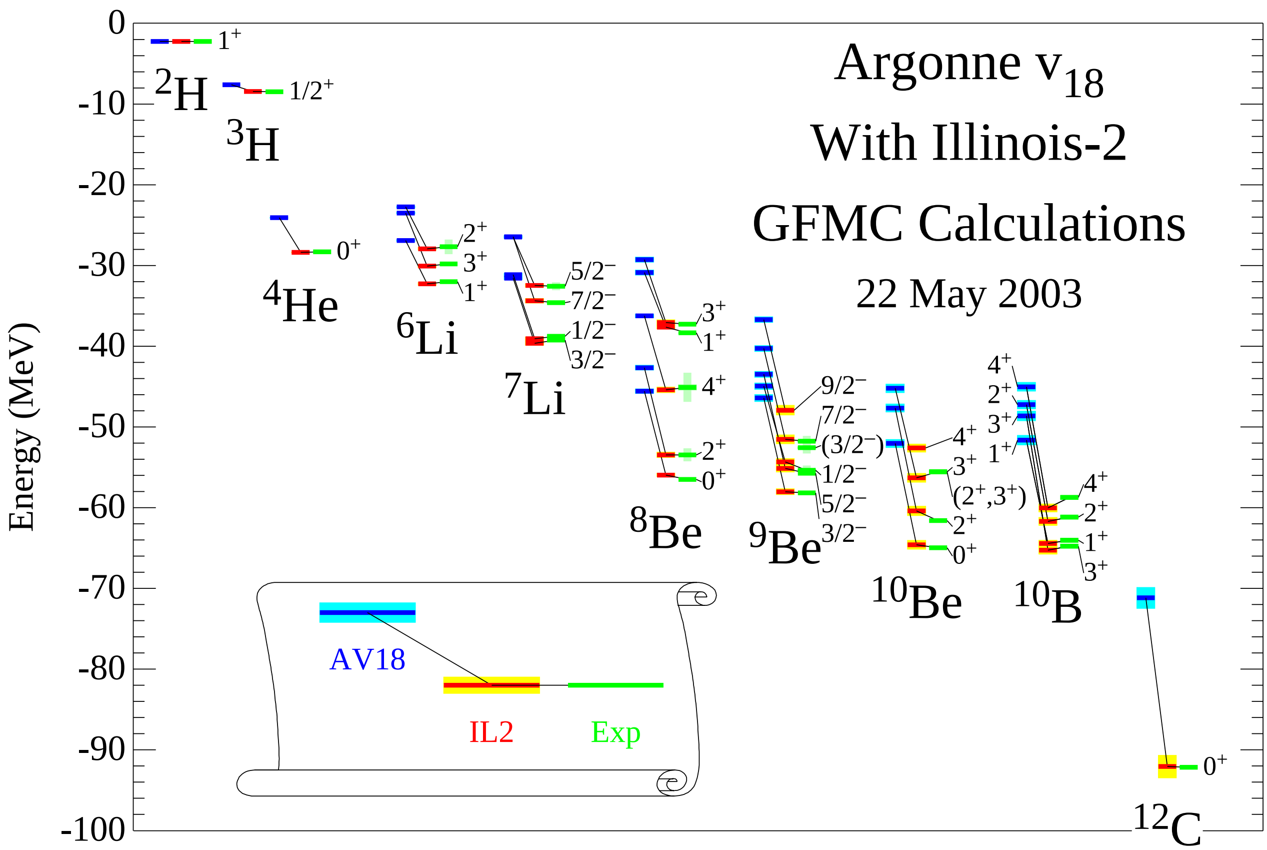
Typical Current Calculations

- Propagation to $\tau = 0.2 - 0.4$ MeV^{-1}
- $E(\tau)$ every $\tau = 0.01$ MeV^{-1} (0.02 for $A \geq 9$)
- Average of $E(\tau)$ for $\tau \geq 0.1$

	Configurations	$\tau_{\rm max}$ MeV^{-1}	Statistical Error (MeV)	Processor hours*
^{6}Li	50,000	0.2	0.08	40
^{8}Li	12,000	0.2	0.2	600
^{9}Be	6,500	0.4	0.5	10,000
^{9}Li	8,000	0.4	0.4	13,500
^{10}B	5,000	0.5	0.5	5,000
^{10}Be	3,000	0.6	0.6	9,000
Preliminary:				
^{12}C	1,400	0.7	1.4	37,500

*6 – 8: IBM SP3 or SGI 250 MHz R10000 processors
9: 500 MHz P-III at ~110 MFLOPS (MCS Chiba)
10: IBM SP at ~320 MFLOPS (NERSC Seaborg)
12: 2.4 GHz P-IV at 616 MFLOPS (Argonne Jazz)

Spectra of Light Nuclei



- AV18: Argonne v_{18} with no $3N$ potential
  - significantly underpredicts experimental values
  - error increases with increasing size of nucleus
- IL2: Argonne v_{18} and Illinois-2 $3N$ potential
  - generally very good agreement with experiment
  - note correct ground-state spin for ^{10}B obtained only with $3N$ potential
- Many other nuclei and levels have been computed
- ^{12}C results are preliminary

^{3}H$(\alpha,\gamma)^{7}$Li & ^{3}He$(\alpha,\gamma)^{7}$Be Capture Reactions

U. of Chicago & Argonne thesis work of Ken Nollett

Source of ^{7}Li in the big bang

- Astrophysically important region is 20−500 keV.

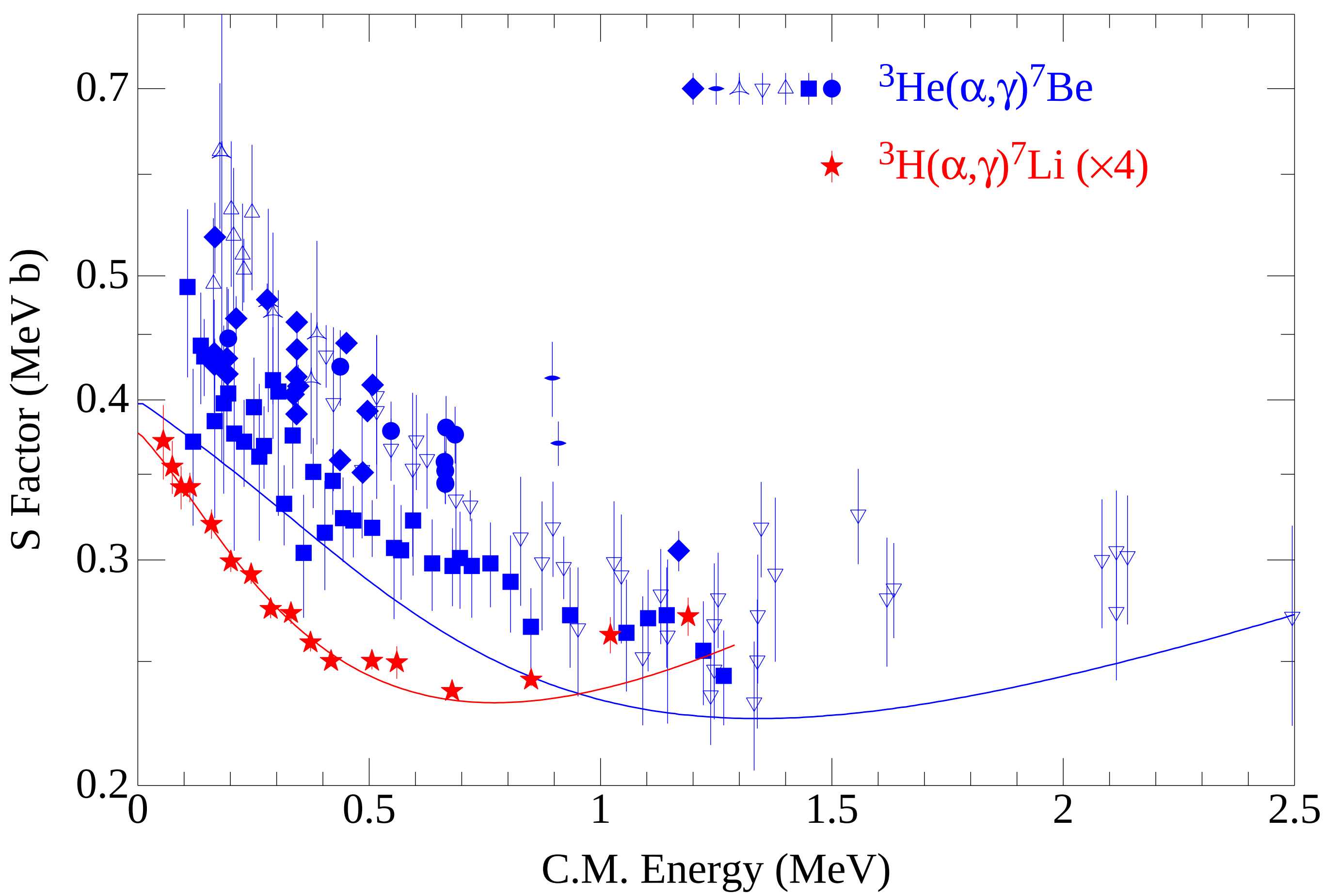
^{7}Be reaction also source of solar neutrinos

- Astrophysically important region is 20 keV.
- No data in this region

Full 7-nucleon calculation

- $A = 7$ wave functions have proper 3+4 cluster form.

^{2}H$(\alpha,\gamma)^{6}$Li also done



Conclusions and Outlook

- New computers and methods allow $\sim 1 - 2\%$ calculations of light p-shell nuclear energies
- Modern nuclear force models give average binding-energy errors < 0.7 MeV for $A = 3 - 10$ nuclei
- Many other nuclear properties can be computed, including experimentally difficult or inaccessible astrophysical reactions.
- GFMC for scattering states – widths of resonances
- ^{12}C by GFMC – May need ~250,000 NERSC CPU hours (600,000 charge hours) for one complete calculation.

We are approaching a nuclear standard model for computing nuclear properties and reactions

GFMC calculations are the benchmark for $6 \leq A \leq 10$