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 \( v_{18} \)

\( v_{ij} = v_{ij}^\gamma + v_{ij}^{CI} + v_{ij}^{CD} ; \quad v_{ij}^{CI} = \sum_{p=1,14} v_p(r_{ij}) O_{ij}^p \)

\[ O_{ij}^p = [1, \sigma_i \cdot \sigma_j, S_{ij}, L \cdot S, L^2, L^2\sigma_i \cdot \sigma_j, (L \cdot S)^2] \otimes [1, \tau_i \cdot \tau_j] \]

\( V_{ijk} \): 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 3\( A - 3 \) variables

(number of isospin states can be reduced)

\( ^{12}\text{C} \): 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:

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

$U_{ijk}$ 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

$\Phi$ 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**: $\Psi_T$ propagated to imaginary time $\tau$:

$$\Psi(\tau) = e^{-(H-E_0)\tau} \Psi_T$$

$$\Psi_0 = \lim_{\tau \to \infty} \Psi(\tau)$$

$$\mathcal{H} \Psi_0 = E_0 \Psi_0$$

**Small time-step propagator**:

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

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

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

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

**Fermion sign problem limits maximum $\tau$**:

$G$ 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

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

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% efficiency 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 $\tau \geq 0.1$

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

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

Argonne $v_{18}$
With Illinois-2
GFMC Calculations
22 May 2003

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

U. of Chicago & Argonne thesis work of Ken Nollett

Source of $^7\text{Li}$ in the big bang
- Astrophysically important region is 20–500 keV.

$^7\text{Be}$ 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.

$^2\text{H}(\alpha, \gamma)^6\text{Li}$ 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 \( \sim 250,000 \) 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 \( 6 \leq A \leq 10 \)