Green's Function Monte Carlo

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The nucleon-nucleon interaction

Nucleon-nucleon interactions are different with respect spin/isospin independent forces, as they depend non only upon the distance between particles, but also on their relative state.

A 'central' or 'scalar' interaction like the Coulomb between electrons, or Lennard-Jones between atoms, do not change the spin, i.e.:

$$\langle s_i s_j | V(r) | s_i' s_j' \rangle = V(r) \delta_{s,s'}$$

The nuclear case is different, it changes the spin/isospin of particles!

Example: Minnesota interaction:

$$V_{ij} = v_c(r_{ij}) + v_\tau(r_{ij}) \tau_i \cdot \tau_j + v_\sigma(r_{ij}) \sigma_i \cdot \sigma_j + + v_{\sigma\tau}(r_{ij}) \sigma_i \cdot \sigma_j \, \tau_i \cdot \tau_j$$

that can be written as:

$$V_{ij} = v_{S=0,T=0}(r) + v_{S=1,T=0}(r) + v_{S=0,T=1}(r) + v_{S=1,T=1}(r)$$

The nucleon-nucleon interaction

What is the problem?

The interaction above, when acting for example on a singlet-spin state generates also a triplet-one:

$$\sigma_i \cdot \sigma_j = 2P_\sigma - 1$$

Then:

$$\sigma_i \cdot \sigma_j |S=0\rangle = \alpha |S=0\rangle + \beta |S=1\rangle$$

One possible solution is to include all the spin/isospin states in the wave function!

The spin/isospin part of the wave function

The wave function can be written as a vector, and each component is an amplitude of a particular spin configuration. For example (three-neutrons):

$$\psi = \begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ a_{\uparrow\uparrow\downarrow} \\ a_{\uparrow\downarrow\uparrow} \\ a_{\uparrow\downarrow\downarrow} \\ a_{\downarrow\uparrow\uparrow} \\ a_{\downarrow\uparrow\downarrow} \\ a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix}$$

The spin/isospin part of the wave function

Then:

$$\sigma_1 \cdot \sigma_2 \Psi = \begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ a_{\uparrow\uparrow\downarrow} \\ 2a_{\downarrow\uparrow\uparrow} - a_{\uparrow\downarrow\uparrow} \\ 2a_{\downarrow\uparrow\downarrow} - a_{\uparrow\downarrow\downarrow} \\ 2a_{\uparrow\downarrow\uparrow} - a_{\downarrow\uparrow\uparrow} \\ 2a_{\uparrow\downarrow\downarrow} - a_{\downarrow\uparrow\downarrow} \\ a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix}$$

$$\sigma_2 \cdot \sigma_3 \Psi = \begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ 2a_{\uparrow\downarrow\uparrow} - a_{\uparrow\uparrow\downarrow} \\ 2a_{\uparrow\uparrow\downarrow} - a_{\uparrow\downarrow\uparrow} \\ a_{\uparrow\downarrow\downarrow} \\ a_{\downarrow\uparrow\uparrow} \\ 2a_{\downarrow\downarrow\uparrow} - a_{\downarrow\uparrow\downarrow} \\ 2a_{\downarrow\uparrow\downarrow} - a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix} \quad ; \quad \sigma_3 \cdot \sigma_1 \Psi = \begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ 2a_{\downarrow\uparrow\uparrow} - a_{\uparrow\uparrow\downarrow} \\ a_{\uparrow\downarrow\uparrow} \\ 2a_{\downarrow\downarrow\uparrow} - a_{\uparrow\downarrow\downarrow} \\ 2a_{\uparrow\uparrow\downarrow} - a_{\downarrow\uparrow\uparrow} \\ a_{\downarrow\uparrow\downarrow} \\ 2a_{\uparrow\downarrow\downarrow} - a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix} .$$

The spin/isospin part of the wave function

How do we do in practice?

Write the spin-isospin part as

$$|\Psi\rangle = \sum_{ij} \psi_{ij}(R)|\chi_\sigma(i)\rangle|\chi_\tau(j)\rangle$$

A convenient way to keep track of all the states is the following:

Example, 4 nucleons, label spin-states as

$$\begin{aligned}
\downarrow_4\downarrow_3\downarrow_2\downarrow_1 &= 0000 = 0 \\
\downarrow_4\downarrow_3\downarrow_2\uparrow_1 &= 0001 = 1 \\
\downarrow_4\downarrow_3\uparrow_2\downarrow_1 &= 0010 = 2 \\
\downarrow_4\downarrow_3\uparrow_2\uparrow_1 &= 0011 = 3 \\
\downarrow_4\uparrow_3\downarrow_2\downarrow_1 &= 0100 = 4 \\
&\dots \\
\uparrow_4\uparrow_3\uparrow_2\downarrow_1 &= 1110 = 14 \\
\uparrow_4\uparrow_3\uparrow_2\uparrow_1 &= 1111 = 15
\end{aligned}$$

The spin/isospin part of the wave function

The charge is conserved. Example, 4 nucleons, for isospin is a bit different:

$$
\begin{aligned}
n_4 n_3 p_2 p_1 &= 1 \\
n_4 p_3 n_2 p_1 &= 2 \\
n_4 p_3 p_2 n_1 &= 3 \\
p_4 n_3 n_2 p_1 &= 4 \\
p_4 n_3 p_2 n_1 &= 5 \\
p_4 p_3 n_2 n_1 &= 6
\end{aligned}
$$

Need to keep a transition table from index (right column) to states (left column).

Then write subroutines to calculate things like $\sigma_i \cdot \sigma_j$, etc.

In practice...

An example:

$$\sigma_i \cdot \sigma_j |\Psi\rangle = (2P_\sigma(i,j) - 1)\,|\Psi\rangle$$

```
  subroutine sigdotsig(wfout,wfin,i,j)
  complex,dimension(0:nspin,ntau) :: wfout,wfin

  do is=0,nspin
! exchange spins i and j in is, store in iex
    iex=ispex(is,i,j)

    wfout(is,:)=2*wfin(iex,:)-wfin(is,:)
  enddo

  end subroutine
```

The nuclear wave function

The correlations now can be spin/isospin dependent:

$$|\Psi\rangle = \mathcal{S} \prod_{i<j} \left[f_c(r_{ij}) + f_\tau(r_{ij}) \tau_i \cdot \tau_j + f_\sigma(r_{ij}) \sigma_i \cdot \sigma_j + \dots \right] |\Phi\rangle$$

Note, the symmetrizer operator $\mathcal{S}$ costs order $\sim N!$, then the order of the pairs is sampled.

Note, in this case $\Psi(R)$ is not a number, but a vector!!!

As explained before, use the above wave function to construct the weight:

$$W(R) = \langle R|\Psi\rangle_l \langle \Psi|R\rangle_r$$

Observables calculated as usual.

Question: why $|\Psi\rangle_l$ and $|\Psi\rangle_r$?

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Question: why $|\Psi\rangle_l$ and $|\Psi\rangle_r$?
Because the sampled order of pairs might be different!

Constrained-path

In the nuclear case Ψ is typically complex, but the weight must be positive and real.

$$W(R) = |\langle R|\Psi\rangle_l \langle\Psi|R\rangle_r|$$

The sign problem is avoided using the **constrained-path** approximation:

Project $\Psi(R)$ on the real axis, and then do not allow its real part to change sign. Then keep the walker only if

$$Re\{\Psi(R')\} * Re\{\Psi(R)\} > 0$$

Note: this approximation **does not** provide an upperbound like in the case of fixed-node!!!

Also in this case the unconstrained-path evolution can be done (similarly to the transient estimate discussed in lecture # 4).

Variational wave function

The number of the total spin (and isospin) states can be reduced by considering appropriate symmetries, but their number is huge:

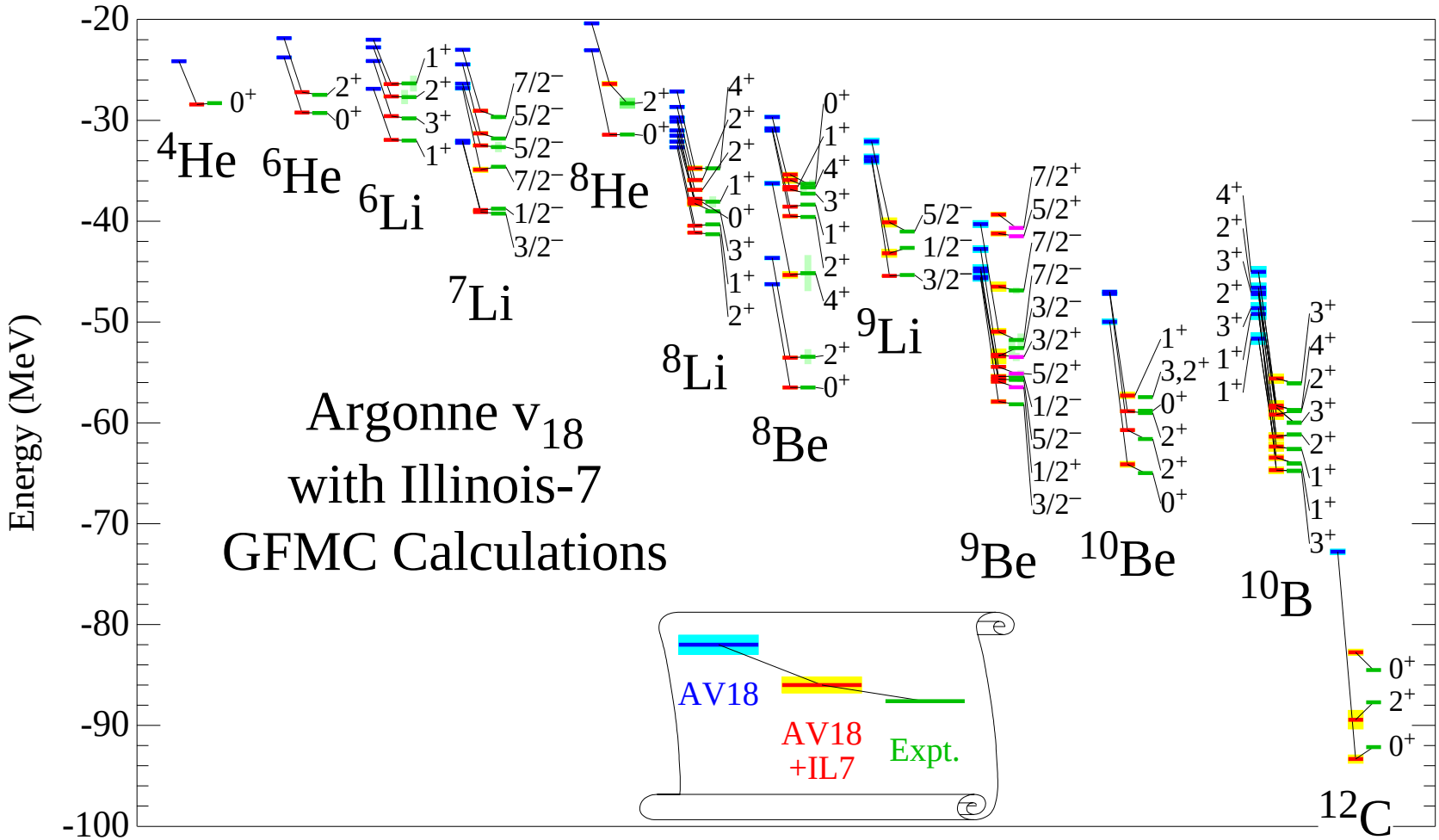
$$\# \approx \frac{A!}{Z!(A-Z)!} 2^A$$

For example:

	A	Pairs	Spin $\times$ Isospin
^{4}He	4	6	8×2
^{6}Li	6	15	32×5
^{7}Li	7	21	128×14
^{8}Be	8	28	128×14
^{9}Be	9	36	512×42
^{10}Be	10	45	512×90
^{11}B	11	55	2048×132
^{12}C	12	66	2048×132
^{16}O	16	120	32768×1430
^{40}Ca	40	780	$3.6 \times 10^{21} \times 6.6 \times 10^{9}$
^{8}n	8	28	128×1
^{14}n	14	91	8192×1

The VMC using this ψ_T provides very accurate results, but it is strongly limited to light systems.

Spectrum of light nuclei



Carlson, et al., Rev. Mod. Phys. 87, 1067 (2015)

Also radii, densities, matrix elements, ...

Monte Carlo integration

Questions???

... for now :-)