Outline

- Notes on Coding and Implementation
- Fixed Node: Implementation
- Fixed Node: Upper Bound
- Transient Estimation: Implementation
- Transient Estimation: Upper Bound(?)
- Transient Estimation: Example
- Multi-Component Wave Functions
- Fixed-Phase Algorithm
- after the break ... VMC for Nuclear Physics

Coding and Implementation

Coding and Implementation

"The print statement is your friend."

Coding and Implementation

(Very) Useful gfortran options

- -O0 -g (-Og) : turns off all bounds checking and enables debugger (slow)
- -Wall : enable all warnings
- -fbounds-check : check indices on arrays to see they are within bounds
- -ffpe-trap=invalid,zero,overflow -g: stops at first invalid math operation
- -O2 or -fast : optimize the code to be fast (when it is working)

Other useful software:

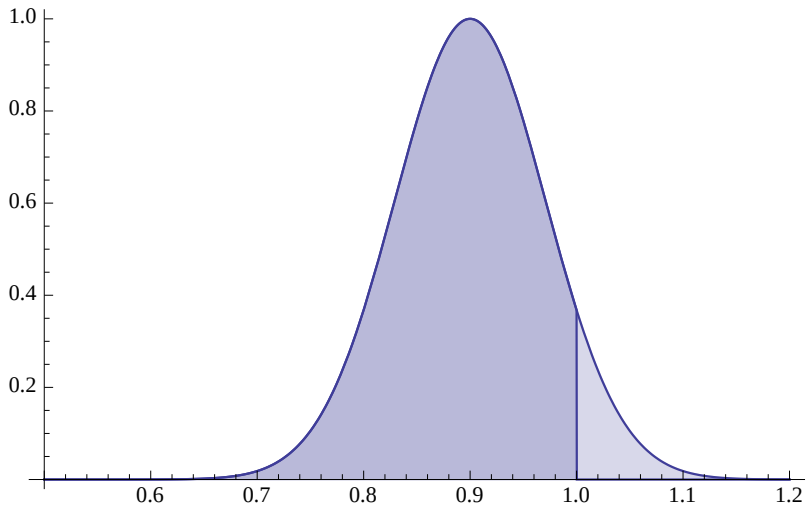
- gdb : simple command-line debugger
- ddd : interface to gdb or other command line debuggers

QMC Implementation

- Print out walk statistics: Acceptance Ratio (VMC), Branching (DMC)
- Keep statistics on several estimators: $< T >$, $< V >$, $< r^2 >$, ...
- Write out walkers at the end of the run
- Have an option to read in these walkers for the next run
- Start DMC from VMC configurations (necessary for TE upper bound... see today)
- Write out block averages to a file for later reanalysis
- Enables a simple code to check for statistics with different blocking

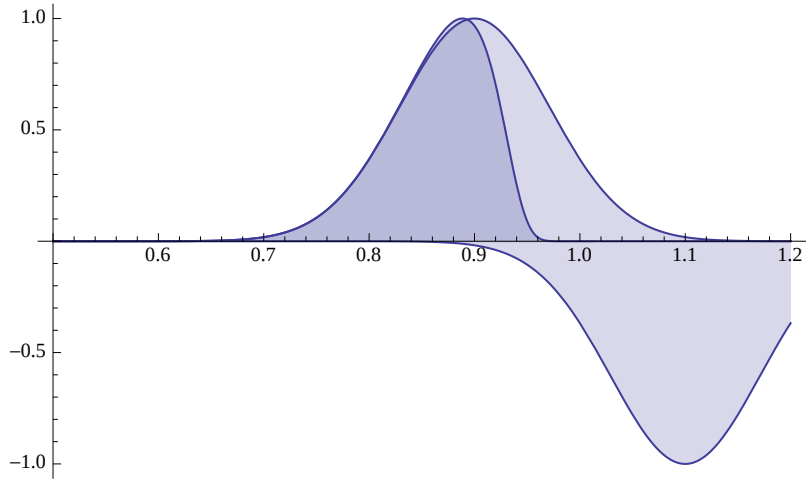
Fixed Node: Implementation

- Last time we described Fixed Node as not letting the walkers move from one sign region to the other
- The simplest implementation is just to 'kill' (set the weight to zero) for any such walker



Fixed Node: Implementation

- This implementation works, but has an error of order $\sqrt{\delta\tau}$
- To improve, subtract an image in the propagator when you are near the node
- This same image method works to enforce logarithmic boundary conditions for low-energy scattering



$$G_{0,FN}(\mathbf{x},\mathbf{x}') = G_0(\mathbf{x},\mathbf{x}') - G_0(\mathbf{x},\mathbf{x}'_{imag})$$

Calculate the image position $\mathbf{x}'$ by a linear extrapolation of :

$$\Psi_T(\mathbf{x}') = \psi_T(\mathbf{x}) + (\mathbf{x}'-\mathbf{x})\nabla\Psi_T(\mathbf{x})$$

Fixed Node as Upper Bound

Why is the fixed node solution an upper bound to the energy?

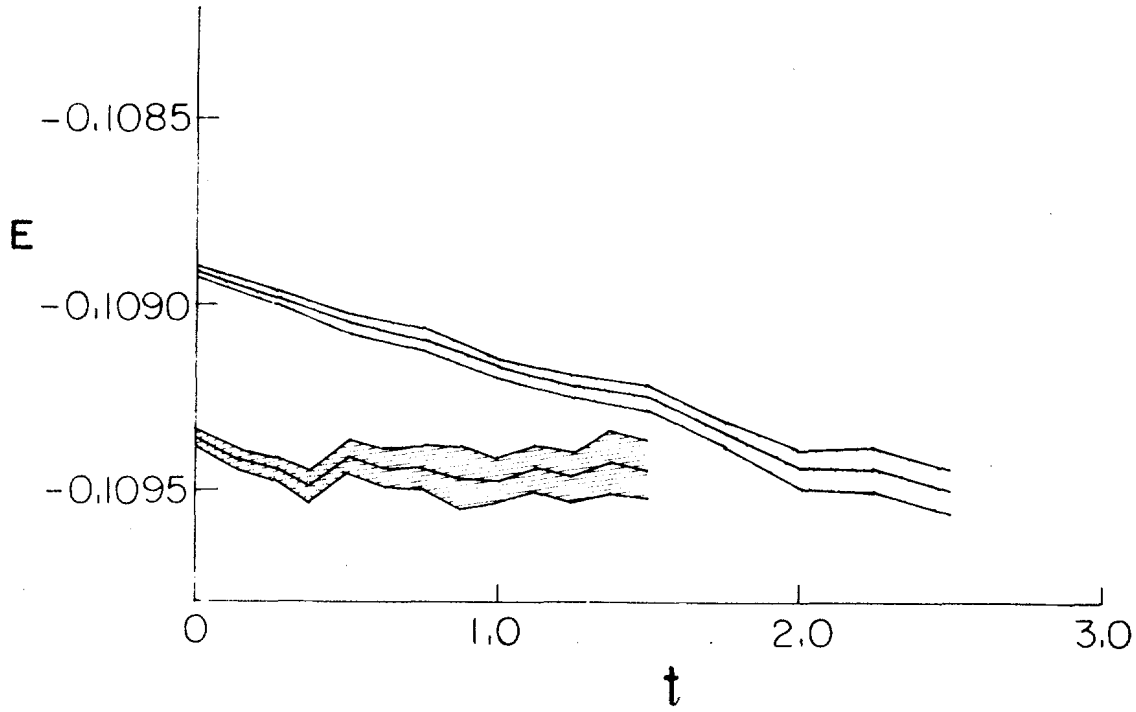
- The fixed node solution Ψ_{FN} is the ground state of a Hamiltonian with an infinite potential at the nodal surface.
- Ψ_{FN} is therefore an eigenstate of this Hamiltonian H_{FN}
- Ψ_{FN} a discontinuous first derivative at the node
- The expectation value of the original Hamiltonian $\langle \Psi_{FN} | H | \Psi_{FN} \rangle$ must provide an upper bound
- Everywhere but at the surface, $H = H_{FN}$.
- The discontinuous derivative yields a delta function in the 2nd derivative of Ψ_{FN},
  but this gives no contribution since Ψ_{FN} is zero there.
- Therefore $E_{FN} \geq E_0$.

Transient Estimation

- We can improve on the fixed-node energy by removing the fixed-node condition.
- Start with a FN simulation with a importance function ψ_G that does not go to zero at the boundary
- Estimators are
$\langle O \rangle = \langle \frac{\langle \Psi_T | O | \Psi \rangle}{\langle \Psi_G | \Psi \rangle} \rangle \; / \; \langle \frac{\langle \Psi_T | \Psi \rangle}{\langle \Psi_G | \Psi \rangle} \rangle$
- This same importance function can be used when we 'release' the fixed node, allowing walkers to pass through the surface.
- If we start from VMC calculations we can get an upper bound to the energy
- Starting from fixed-node we do not have an upper bound property

Electron Gas

One of the most-cited papers ever (in any field): (top 5?)



Electron gas: Transient estimation from fixed node and from VMC (Ceperley, PRL, 1980). This paper had a huge impact because it is widely used in density functional theories for electronic systems.

Multi-Component Wavefunctions

In many systems the wave function cannot be described as a single number for each position of the particles. Examples include:

- Nuclear Systems : different spin and isospin components (each complex)
- Vortices: Complex wave function describing the rotation
- Magnetic Field: electrons in a magnetic field (complex wave function

Simplest Fixed Phase

Take the simplest example with a complex wave function: $\Psi = |\Psi| \exp[i\Phi(R)]$, We can create an algorithm that solves for the optimum $|\Psi(R)|$ given the phase $\Phi(R)$. The equation for $|\Psi|$ is

$$-\nabla^2|\Psi(R)| + [V(R) + |\nabla\Phi(R)|^2]|\Psi(R)| = E|\Psi(R)|$$

This is the same as the standard Schroedinger equation with an 'extra' potential from the gradient of the phase squared. This is a 'bosonic' problem and produces a variational upper bound. It reduces to the fixed node in the case that the phase changes infinitely quickly from -1 to 1.

Fixed phase was first introduced in nuclear systems with multi-component wave functions. It can be implemented to have an upper bound property in some cases, while simultaneously providing an upper bound.

Nuclear Case

In nuclei, there are many possible spin isospin states in the system, ranging from all spins down to all spins up, for a total of 2^A states. There are a similarly large number of isospin states, though these are limited by charge conservation (and isospin conservation if we ignore Coulomb and other smaller isospin-violating interactions).
We can write:

$$|\Psi\rangle = \sum_i |\psi_i(R)\rangle|\chi_i\rangle. \tag{1}$$

The norm of the wave function is:

$$\langle\Psi|\Psi\rangle = \int d\mathbf{R} \sum_i \psi^\dagger(\mathbf{R})\psi(\mathbf{R})\langle\chi_i|\chi_i\rangle, \tag{2}$$

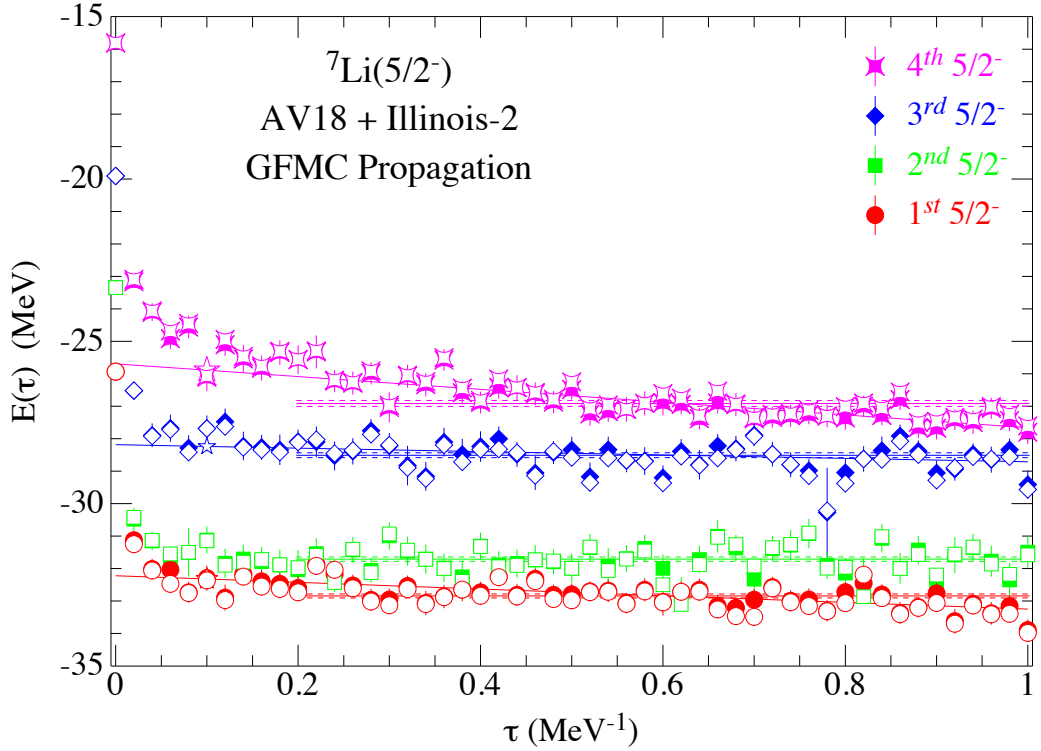
assuming the χ_i form an orthonormal basis.
The energy of the wave function is

$$\langle\Psi_i|H|\Psi_j\rangle = \int d\mathbf{R} \sum_i \sum_j \psi^\dagger(\mathbf{R})\langle\chi_i|H_{ij}|\chi_j\rangle|\psi(\mathbf{R})\rangle,$$

where the potential can couple different i, j states.

Nuclear Case

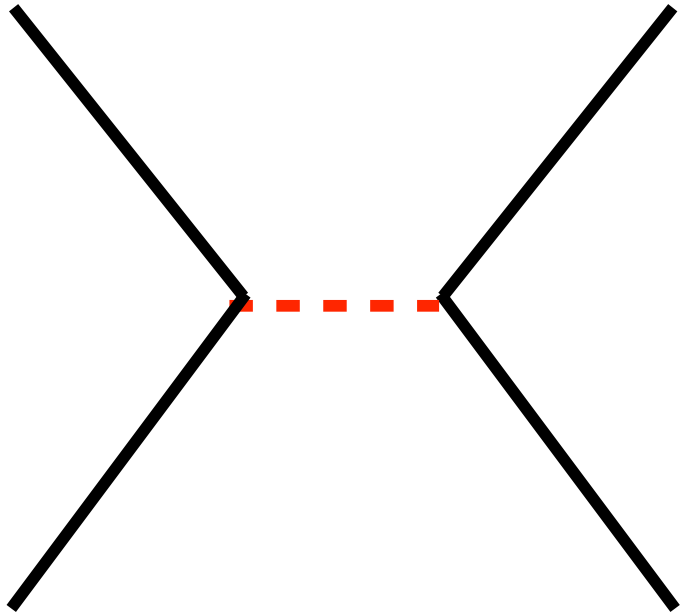
Calculations of different states in A=7



- Different States converge at different rates
- Bound States have a finite gap; converge with respect to typical excitation energy
- Very narrow states are similar but decrease very slowly
- Broad Scattering states should eventually go to isolated clusters

How do we calculate Nuclei?

Nucleon-Nucleon interactions are unlike Coulomb interactions or many inter-atomic potentials in that they change the spin and/or isospin of the particles.



$$V^{\pi} = -\frac{g_A}{\sqrt{2}f_\pi}\frac{\sigma_i\cdot\mathbf{q}\sigma_j\cdot\mathbf{q}}{q^2+m_\pi^2}\tau_i\cdot\tau_j$$

For example, the charge of a neutron and proton can be exchanged by the propagation of a charged pion. In general the wave function must be written as a sum of complex spin-isospin amplitudes.

Simple Potential: Minnesota interaction

For the problems, we consider an interaction that has four components:

$$V_{ij} = V^1(r_{ij}) \; + \; V^\sigma(r_{ij}) \; + \; V^\tau(r_ij) + V^{\sigma\tau}(r_{ij}).$$

- This is a significant simplication, no tensor interaction
- The matrix elements are purely real
- The interaction is very attractive in T=0,S=1 and S=1,T=0 (s-wave) pairs
- The interaction is weaker in p-waves
- This type of interaction can be used in pionless EFT

Basic Idea for VMC

The basic idea is to write the wave function as a set of amplitudes

$$|\Psi\rangle \;=\; \sum_{i,j} \psi_{i,j}(\mathbf{R})\; |\chi^{\sigma}(i)\rangle\; |\chi^{\tau}(j)\rangle,$$

and use the sum of the squares of the amplitudes to calculate probabilities for the random walk.

$$W(\mathbf{R}) \;=\; \sum_{i,j} \psi^{\dagger}(\mathbf{R})\; \psi(\mathbf{R})$$

The expectation value of the Hamiltonian is obtained as averages over:

$$\langle H \rangle \;=\; \frac{\langle \frac{\langle \psi^{\dagger}_{i,j} \langle \chi^{\sigma}(i)\chi^{\tau}(j)|\;\; H \;\; |\psi_{i,j}|\chi^{\sigma}(i)\chi^{\tau}(j)\rangle}{W(\mathbf{R})} \rangle}{\langle \frac{\langle \psi^{\dagger}_{i,j} \langle \chi^{\sigma}(i)\chi^{\tau}(j)|\psi_{i,j}|\chi^{\sigma}(i)\chi^{\tau}(j)\rangle}{W(\mathbf{R})} \rangle},$$

where the brackets in the numerator and denominator indicate separate averages.

Pauli Spinor Matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_+ = (1/2)(\sigma_x + i\sigma_y) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$\sigma_- = (1/2)(\sigma_x - i\sigma_y) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$\sigma.\mathbf{A} = \sigma_+ \cdot (\mathbf{A}_x - i\mathbf{A}_y) + \sigma_- \cdot (\mathbf{A}_x + i\mathbf{A}_y) + \sigma_z \cdot \mathbf{A_z}$$

Spin States

The spin state are:

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

Isopin States

The isospin state are:

$$
\begin{array}{lcll}
n_4 n_3 p_2 p_1 & = & 0011 & = 1 \\
n_4 p_3 n_2 p_1 & = & 0101 & = 2 \\
n_4 p_3 p_2 n_1 & = & 0110 & = 3 \\
p_4 n_3 n_2 p_1 & = & 1001 & = 4 \\
p_4 n_3 p_2 n_1 & = & 1010 & = 5 \\
p_4 p_3 n_2 n_1 & = & 1100 & = 6
\end{array}
$$

Keep a translation table translating from index (right column) to bit representation, use that to calculate matrix elements.

Variational Monte Carlo: $|\Phi\rangle$

In Variational Monte Carlo, we again assume a simple structure for the trial wave function:

$$|\Psi_T\rangle \;=\; [\mathcal{S}\prod_{i<j} F_{ij}]|\Phi\rangle$$

For A=3,4 we can use a very simple $|\Phi\rangle$ that contains only spin-isospin states, e.g.

$$|\Phi\rangle \;=\; \mathcal{A}|\uparrow_4 p_4 \downarrow_3 p_3 \uparrow_2 n_2 \downarrow_1 n_1\rangle$$

For the α particle this is a sum of 24 terms.
For larger nuclei a shell-model like state or states can be used.
Computations can become very time-consuming because of the explicit anti-symmetrization usually invoked to introduce clustering.

Uncorrelated State $|\Phi\rangle$

$|\Phi\rangle = \mathcal{A} \downarrow_4 n_4 \uparrow_3 n_3 \downarrow_2 p_2 \uparrow_1 p_1$ This is independent of coordinates (for A $<$ 5) and never changes

```
    3     2 -0.1000000E+01  0.0000000E+00
    3     3  0.1000000E+01  0.0000000E+00
    3     4  0.1000000E+01  0.0000000E+00
    3     5 -0.1000000E+01  0.0000000E+00
    5     1  0.1000000E+01  0.0000000E+00
    5     3 -0.1000000E+01  0.0000000E+00
    5     4 -0.1000000E+01  0.0000000E+00
    5     6  0.1000000E+01  0.0000000E+00
....
    6     1 -0.1000000E+01  0.0000000E+00
    6     2  0.1000000E+01  0.0000000E+00
   12     5 -0.1000000E+01  0.0000000E+00
```

VMC: Two-Body Operations

For the potential or for the most general pair correlation operator we construct an output wave function for an operator acting on an input wae function:

$$|\Psi_o\rangle = \sum_k f^k(r_{ij})|\Psi_i\rangle$$

The f_k are simple numbers for a given set of coordinates, the operators $O^k(r_{ij})$ are sparse matrices acting on the intial state.

We operate in succession by all pair operators gradually building up the full correlated wave function.

Simple Example

We will ask you to consider a simple problem where the variational wave function is:

$$|\Psi\rangle \;=\; \prod_{i<j} F^c(r_{ij})]|\Phi\rangle$$

Here the derivatives act only on the central pair correlation functions and the spin-isospin structure of the trial function is fixed.

We still need to determine spin isospin operators acting on the trial state to calculate the potential energy.

Simple Example (cont'd)

To calculate the matrix elements of $\sigma_i \cdot \sigma_j$ in a many-particle system, remember

$$\sigma_i \cdot \sigma_j = 2P^\sigma(i,j) - 1,$$

where P is the spin permutation operator. To calculate this, just store the state obtained by $P^\sigma(i,j)$ acting on every initial state. For example

$$\begin{aligned} P(1,2)|1001\rangle &= |1010\rangle \\ P(1,2)|0101\rangle &= |0110\rangle \\ &\cdots \\ P(1,2)|1011\rangle &= |1011\rangle \end{aligned}$$

We need only two matrix elements for each $\sigma_i \cdot \sigma_j$. Similar methods work for the tensor operator and isospin operators. Only two spins or isospins are affected at a time so the matrix is sparse.

Subroutines

All wavefunctions are matrices of dimensions (0:2**A-1,ntau0=6).

- phi_init(): initializes $|\phi\rangle$, all $+/-1$.
- spin_init(n): initializes spin states for n particles
- iso_init(n,nz): initializes isospin states for n particles, nz protons
- covlp(cl,cr): takes overlaps of two wvfns $\langle cl|cr\rangle$
- sigdotsig(co,ci,i,j): computes $|co\rangle = \sigma_i \cdot \sigma_j |ci\rangle$
- taudottau(co,ci,i,j): computes $|co\rangle = \tau_i \cdot \tau_j |ci\rangle$
- sdstdt(co,ci,i,j): computes $|co\rangle = \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j |ci\rangle$

subroutine for $\sigma_i \cdot \sigma_j$ interaction

```
subroutine sigdotsig( cwvout,cwvin,i,j)
complex(kind=kind(0.d0)),dimension(0:nspin0m,ntau0)
do is=0,nspin0m
iex=ispex(is,i,j)  ! exchange spins i and j in is,
cwvout(is,:)= 2.d0*cwvin(iex,:)-cwvin(is,:)
enddo
end subroutine
```

subroutine for $\sigma_i \cdot \sigma_j \tau_i \cdot \tau_j$ interaction

```
      subroutine sdstdt( cwvout,cwvin,i,j)
!       calculate sig . sig tau.tau acting on cwvin store
!       cwvin and cwvout must not overlap
      complex(kind=kind(0.d0)),dimension(0:nspin0m,ntau0)
      do it=1,ntau
      itauex=itex(it,i,j)
      do is=0,nspin0m
      ispinex=ispex(is,i,j)
      cwvout(is,it)= 4.d0*cwvin(ispinex,itauex)-2.d0*cwvi
     &   -2.d0*cwvin(ispinex,it) + cwvin(is,it)
      enddo
      enddo
      end subroutine
```

Simplified Wave function and Local Energy

$$|\Psi\rangle = \prod_{i<j} f^c(|\mathbf{r}_i - \mathbf{r}_j|)|\phi\rangle$$

The local energy is: $\langle T\rangle + \langle V\rangle$

$$\langle T\rangle = \frac{\langle\phi|\left(\prod f\right)\left[-\frac{\hbar^2}{2m}\nabla^2\right]\left(\prod f\right)|\phi\rangle}{\langle\phi|\left(\prod f\right)\left(\prod f\right)|\phi\rangle}$$

$$\langle V\rangle = \frac{\langle\phi|\left(\prod f\right)[\sum_{i<j}[v^c(r_{ij}) + v^\sigma(r_{ij})\sigma_i\cdot\sigma_j + v^\tau(r_{ij})\tau_i\cdot\tau_j + v^{\sigma\tau}(r_{ij}}{\langle\phi|\left(\prod f\right)\left(\prod f\right)|\phi\rangle}$$

Kinetic Energy

The derivatives of the kinetic energy are calculated numerically:

$$-\nabla^2|\Psi\rangle = \sum_i \nabla^2\phi_i|\chi_i\rangle$$

$$= \sum_i -(1/\Delta)^2[\phi_i(+) + \phi_i(-) - 2*\phi_i(0)]|\chi_i\rangle$$

The local kinetic energy is

$$\frac{\sum_i \langle\chi_i\phi_i(0)(1/\Delta)^2[\phi_i(+) + \phi_i(-) - 2*\phi_i(0)\chi_i\rangle}{\sum_i\langle\chi_i\phi_i(0)\phi_i(0)\chi_i\rangle}$$

Variational Monte Carlo

Construct random walk from probability:

$$W = \langle\phi| \left(\prod f^c\right) \left(\prod f^c\right) |\phi\rangle,$$

in real applications we use a better (more complicated wave function) with spin-dependent correlations also. In this case we sample the sum over order of pair operators independently on the right and left. We use a positive definite function of $\langle\Psi_l|\Psi_r\rangle$.

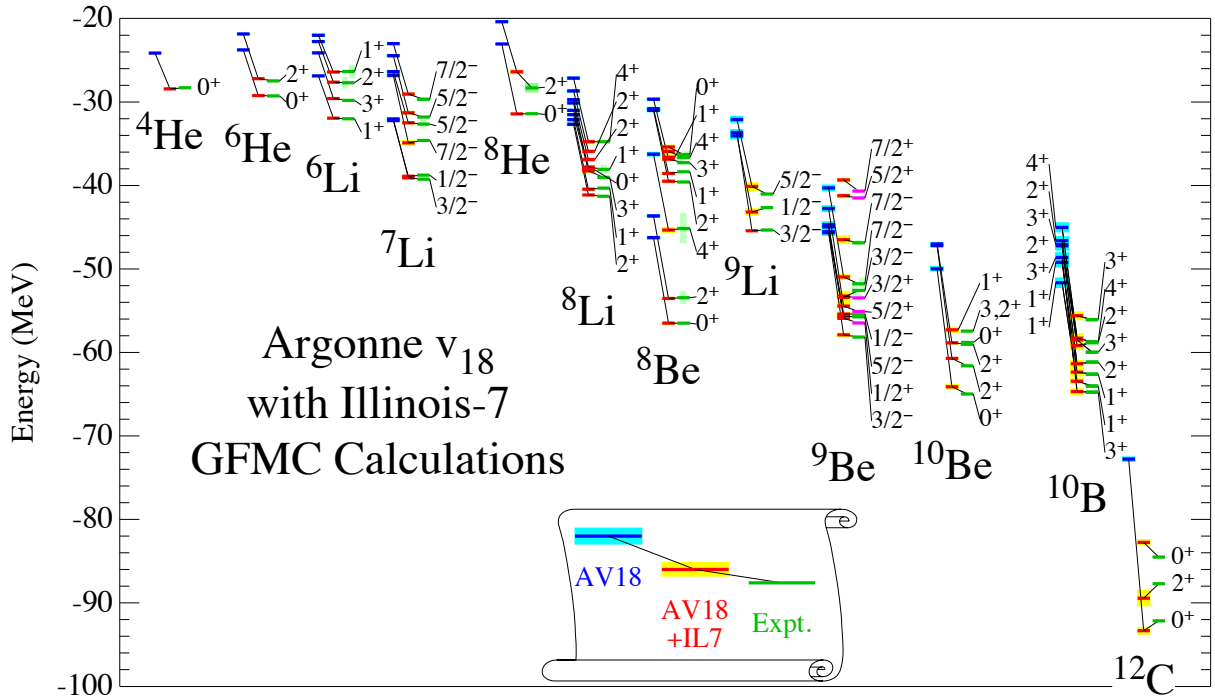
VMC is just as before, calculate probability of a step from the square of the wave function and average the local energy.

DMC for Nuclear Case

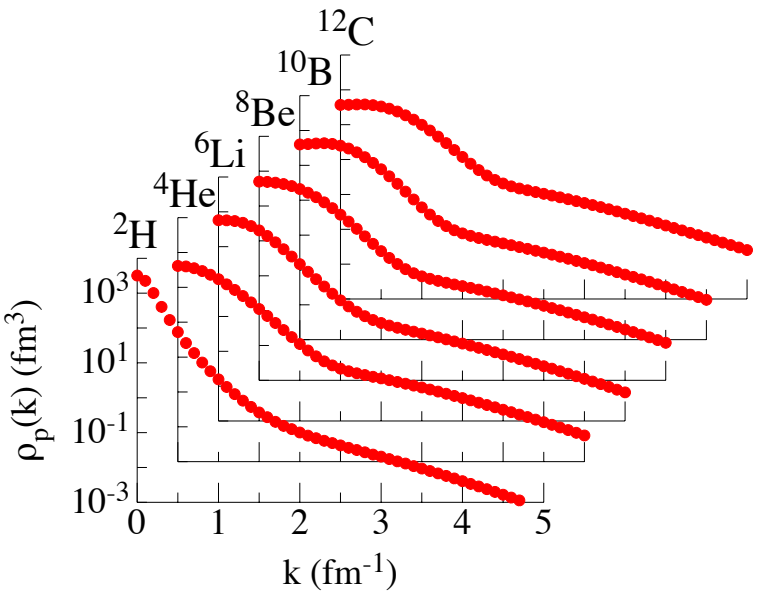
Next Time.....

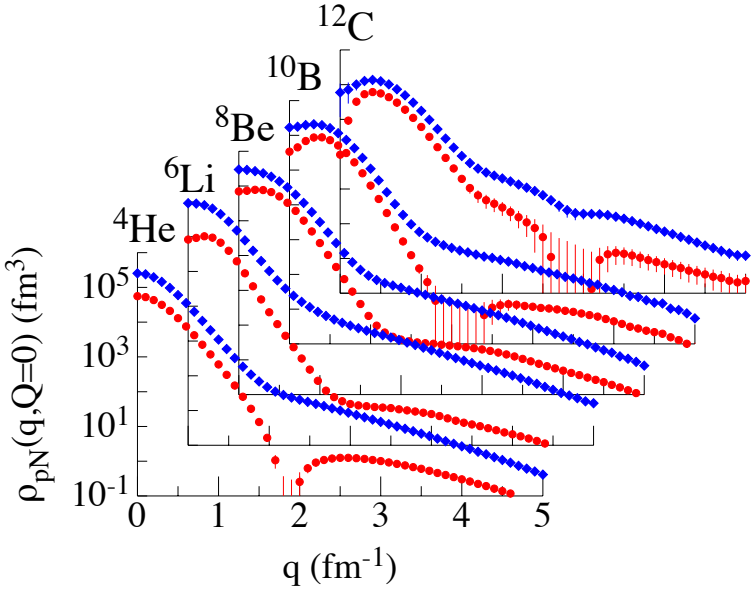
What can we calculate?

Energy Levels

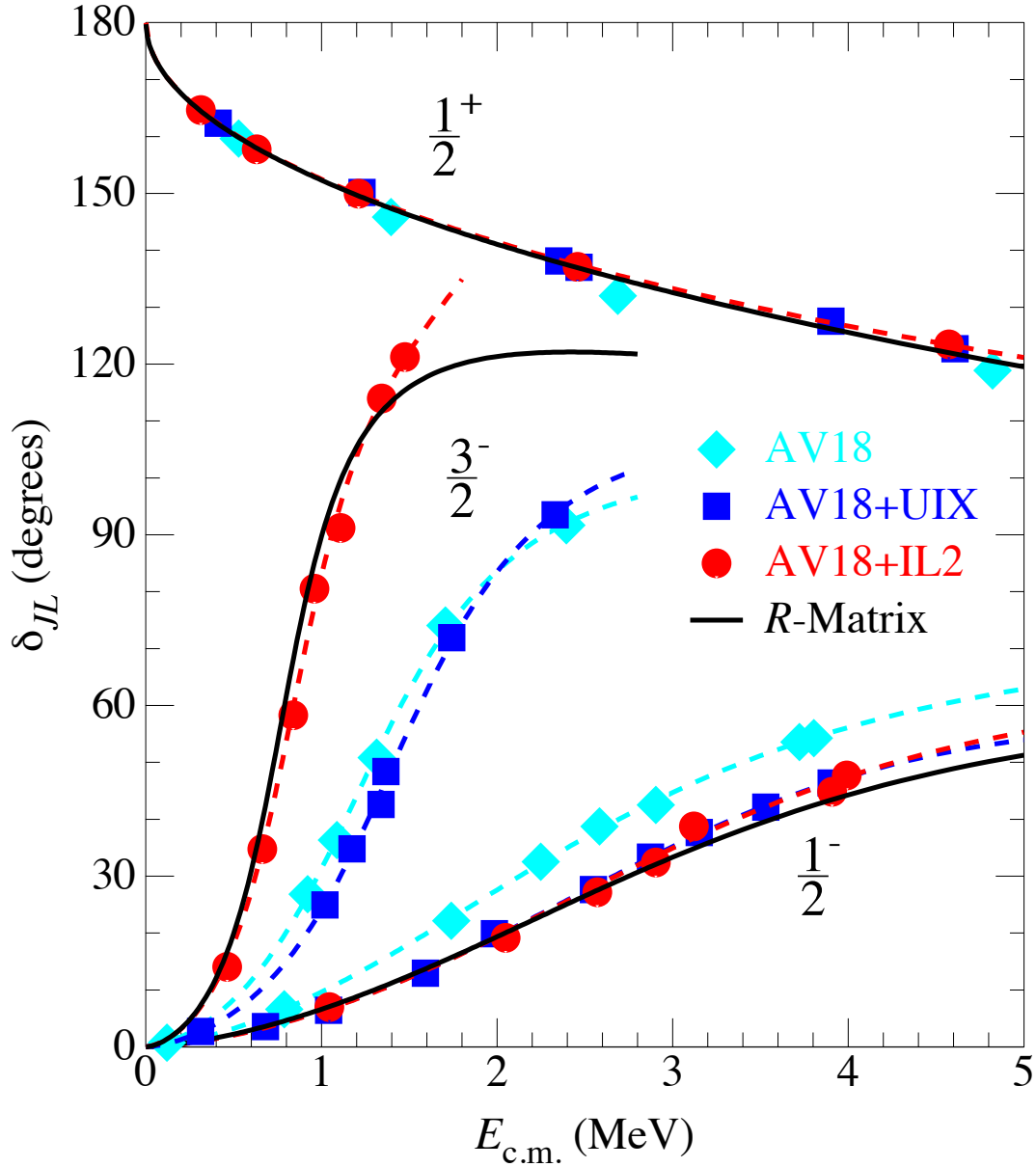


Momentum Distributions

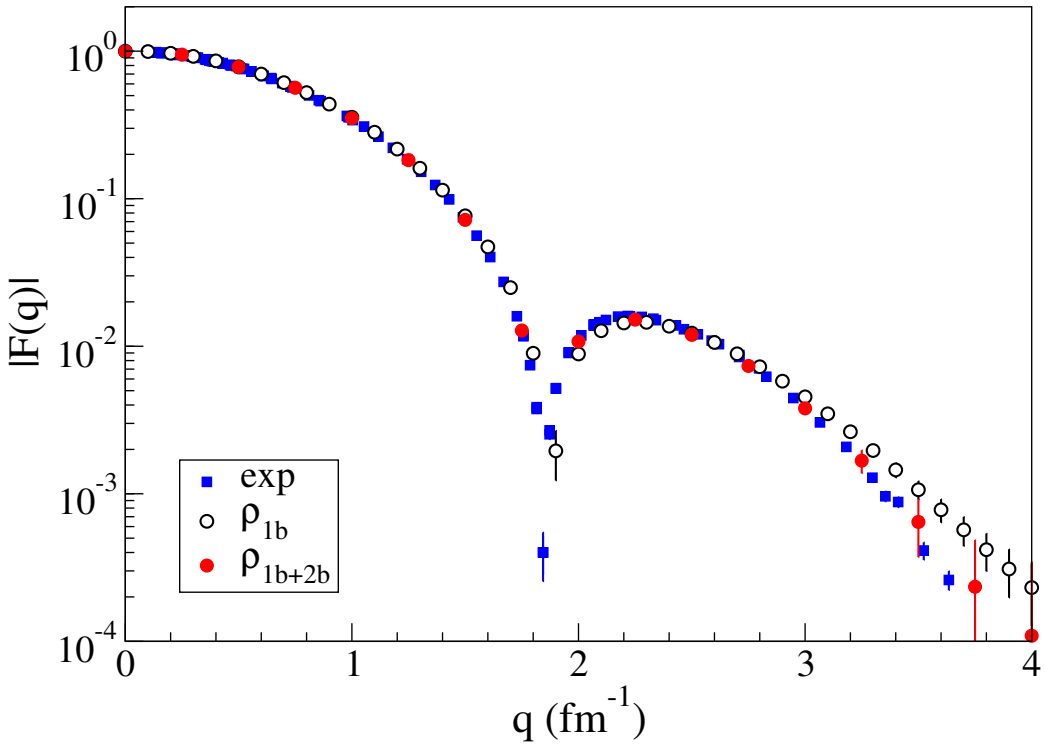




Scattering Phase Shifts



EM Form Factors



Other Quantities

- Magnetic Moments
- M1, E2, and GT transition matrix elements
- electron, neutrino scattering
- ...