Auxiliary Field Diffusion Monte Carlo (II)

Stefano Gandolfi

Los Alamos National Laboratory (LANL)

TALENT School on Nuclear Quantum Monte Carlo Methods
North Carolina State University (NCSU), July 11-29 2016.

Spin-dependent interactions

Remember: define a spinor for each nucleon

$$s_i \equiv \begin{pmatrix} a_i \\ b_i \\ c_i \\ d_i \end{pmatrix} = a_i|p\uparrow\rangle + b_i|p\downarrow\rangle + c_i|n\uparrow\rangle + d_i|n\downarrow\rangle\,,$$

where a_i, b_i, c_i and d_i are complex numbers, and the $\{|p\uparrow\rangle, p\downarrow\rangle, |n\uparrow\rangle, |n\downarrow\rangle\}$ is the proton-up, proton-down, neutron-up and neutron-down basis.

So now each walker contains:

$$W_i = \{\vec{r}_1, s_1, \vec{r}_2, s_2, \ldots \vec{r}_n, s_n\} = \{R, S\}$$

AFDMC wave function

Let's just consider the spin of nucleons. The trial (variational) wave must be antisymmetric under the exchange of pairs. The general (easy) form is:

$$\langle S, R|\Psi_T\rangle = \prod_{i<j} f(r_{ij})\,\mathcal{A}\{\phi_{\alpha_1}(r_1, s_1)\ldots\phi_{\alpha_N}(r_N, s_N)\}$$

where $\phi_n(r, s)$ are single particle orbitals.

The (simple) Jastrow factor is spin-independent, and only depends upon the coordinates of nucleons (as for the scalar case).

AFDMC wave function

The antisymmetric part is constructed as a Slater determinant:

$$\mathcal{A}\{\phi_{\alpha_1}(r_1,s_1)\dots\phi_{\alpha_N}(r_N,s_N)\} = \begin{vmatrix} \phi_1(r_1,s_1) & \phi_1(r_2,s_2) & \dots & \phi_1(r_N,s_N) \\ \phi_2(r_1,s_1) & \phi_2(r_2,s_2) & \dots & \phi_2(r_N,s_N) \\ \dots & \dots & \dots & \dots \\ \phi_N(r_1,s_1) & \phi_N(r_2,s_2) & \dots & \phi_N(r_N,s_N) \end{vmatrix}$$

where the single particle orbitals depend upon the coordinates and the spin of the nucleons, in general:

$$\phi_{\alpha_i}(r_j,s_j) = \langle r_j, s_j|\phi_{\alpha_i}\rangle = \langle \vec{r}_j|f_{n_i}(r)\rangle\,\langle s_j|\xi_i\rangle$$

Example: spin of neutrons

We have two spin states, so:

$$|\xi_1\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad |\xi_2\rangle = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Then the overlap for the nucleon i-th with the $\uparrow$ state is given by:

$$\langle s_i|\xi_1\rangle = (a_i, b_i)\begin{pmatrix} 1 \\ 0 \end{pmatrix} = a_i$$

and for the $\downarrow$ state:

$$\langle s_i|\xi_2\rangle = (a_i, b_i)\begin{pmatrix} 0 \\ 1 \end{pmatrix} = b_i$$

AFDMC wave function

Example: neutrons in a periodic box.
The radial functions in a periodic box are plane waves:

$$\langle \vec{r}_j | \phi_n(r) \rangle = \exp(i\,\vec{k}_n \cdot \vec{r}_j)$$

with momenta

$$\begin{aligned}
\vec{k}_1 &= \frac{2\pi}{L}(0,0,0) \\
\vec{k}_2 &= \frac{2\pi}{L}(1,0,0) \\
\vec{k}_3 &= \frac{2\pi}{L}(-1,0,0) \\
\vec{k}_4 &= \frac{2\pi}{L}(0,1,0) \\
\vec{k}_5 &= \frac{2\pi}{L}(0,-1,0) \\
&\dots
\end{aligned}$$

AFDMC wave function

Then the Slater determinants for $N/2$ nucleons with spin-$\uparrow$, and $N/2$ with spin-$\downarrow$ is:

$$\begin{vmatrix}
a_1 & a_2 & \dots & a_N \\
a_1 \exp(i\frac{2\pi}{L}x_1) & a_2 \exp(i\frac{2\pi}{L}x_2) & \dots & a_N \exp(i\frac{2\pi}{L}x_N) \\
a_1 \exp(-i\frac{2\pi}{L}x_1) & a_2 \exp(-i\frac{2\pi}{L}x_2) & \dots & a_N \exp(-i\frac{2\pi}{L}x_N) \\
a_1 \exp(i\frac{2\pi}{L}y_1) & a_2 \exp(i\frac{2\pi}{L}y_2) & \dots & a_N \exp(i\frac{2\pi}{L}y_N) \\
a_1 \exp(-i\frac{2\pi}{L}y_1) & a_2 \exp(-i\frac{2\pi}{L}y_2) & \dots & a_N \exp(-i\frac{2\pi}{L}y_N) \\
a_1 \exp(i\frac{2\pi}{L}z_1) & a_2 \exp(i\frac{2\pi}{L}z_2) & \dots & a_N \exp(i\frac{2\pi}{L}z_N) \\
a_1 \exp(-i\frac{2\pi}{L}z_1) & a_2 \exp(-i\frac{2\pi}{L}z_2) & \dots & a_N \exp(-i\frac{2\pi}{L}z_N) \\
\dots & \dots & \dots & \dots \\
b_1 & b_2 & \dots & b_N \\
b_1 \exp(i\frac{2\pi}{L}x_1) & b_2 \exp(i\frac{2\pi}{L}x_2) & \dots & b_N \exp(i\frac{2\pi}{L}x_N) \\
\dots & \dots & \dots & \dots
\end{vmatrix}$$

Alpha particle

For the alpha particle the antisymmetric part of the wave function is just spinor dependent with also isospin:

$$
\begin{vmatrix}
\langle s_1|p\uparrow\rangle & \langle s_2|p\uparrow\rangle & \langle s_3|p\uparrow\rangle & \langle s_4|p\uparrow\rangle \\
\langle s_1|p\downarrow\rangle & \langle s_2|p\downarrow\rangle & \langle s_3|p\downarrow\rangle & \langle s_4|p\downarrow\rangle \\
\langle s_1|n\uparrow\rangle & \langle s_2|n\uparrow\rangle & \langle s_3|n\uparrow\rangle & \langle s_4|n\uparrow\rangle \\
\langle s_1|n\downarrow\rangle & \langle s_2|n\downarrow\rangle & \langle s_3|n\downarrow\rangle & \langle s_4|n\downarrow\rangle
\end{vmatrix}
=
\begin{vmatrix}
a_1 & a_2 & a_3 & a_4 \\
b_1 & b_2 & b_3 & b_4 \\
c_1 & c_2 & c_3 & c_4 \\
d_1 & d_2 & d_3 & d_4
\end{vmatrix}
$$

In the code this is simply done as:

```
ph=0.0
ph(1,1,:)=1.0
ph(2,2,:)=1.0
ph(3,3,:)=1.0
ph(4,4,:)=1.0
do i=1,npart
   smati(:,i)=matmul(ph(:,:,i),w%sp(:,i))
enddo
call cmatinv(smati,det,npart) ! calculate the determinant
```

Propagation

We have seen that the full propagator (without importance sampling) is:

$$G(R,R,\delta\tau) = \left(\frac{m}{2\pi\hbar^2\delta\tau}\right)^{\frac{3A}{2}} e^{-\frac{m(R-R')^2}{2\hbar^2\delta\tau}} e^{-V_{SI}(R)\delta\tau} \times \prod_{n=1}^{15A} \frac{1}{\sqrt{2\pi}} \int dx_n e^{-\frac{x_n^2}{2}} e^{\sqrt{-\lambda_n\delta\tau}x_n O_n}$$

Note: for the v_4 and v_6 interaction there are 15 operators for each nucleon, 3 σ, 3 τ, and 9 $\sigma\tau$.

Propagation of spinors

Now, let's see how the propagation (rotation) of spinors works for Minnesota:

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

We first need to rewrite the interaction as:

$$v_{ij} = V_{SI} + \sum_\alpha \sigma_i^\alpha A_{ij}^{(\tau)} \sigma_j^\alpha + \sum_{\alpha\beta} \sigma_i^\alpha \tau_i^\beta A_{ij}^{(\sigma)} \sigma_j^\alpha \tau_j^\beta + \sum_\alpha \tau_i^\alpha A_{ij}^{(\sigma\tau)} \tau_j^\alpha$$

The matrices are calculated as:

```
do j=1,npart
   do i=1,npart
      dx(:)=x(:,i)-x(:,j)
      r=sqrt(dot_product(dx,dx))
      call minnesota(r,ac(i,j),at(i,j),as(i,j),ast(i,j))
   enddo
enddo
```

Propagation of spinors

Given a set of (sampled) auxiliary fields x_n, we have to apply the propagator:

$$\exp\left[\sqrt{-\lambda_n\delta\tau}x_n\sum_\alpha\sum_{j\beta}\tau_{j\alpha}\sigma_{j\beta}\psi_{j\beta}^{(n)}\right]|s_n\rangle =$$

First we need to diagonalize the matrices $A^{(\tau)}$, $A^{(\sigma)}$, and $A^{(\sigma\tau)}$:

```
call eigenrs(atau,valtau,npart)
call eigenrs(asig,valsig,npart)
call eigenrs(asigtau,valsigtau,npart)
```

The above subroutines take a matrix *atau* (and others), and return the eigenvectors stored in the same arrays, and the eigenvalues *valtau*.

Propagation of spinors

$$\exp\left[\sqrt{-\lambda_n\delta\tau}x_n\sum_\alpha\sum_j\tau_{j\alpha}\psi_j^{(n)}\right]|s_n\rangle =$$

Now we have to construct the n-operators $O_n^{(\tau)} = \sum_{j\alpha}\tau_{j\alpha}\psi_j^{(n)}$

```
do n=1,3*npart ! loop over n=1...3*npart
   do is=1,3 ! loop over taux, tauy, tauz
      do i=1,npart ! loop over eigenvectors
         cfac=sqrt(-valtau(n)*dt)
         rott(is,n)=x(n)*cfac*atau(n,i)
      enddo
   enddo
enddo
```

Propagation of spinors

The operators O_n are basically linear combinations of spin and isospin operators multiplied by the eigenvectors ψ. For one spinor the rotation of the spin turns out to be:

$$\begin{pmatrix} \psi_z & \psi_x - i\psi_y & 0 & 0 \\ \psi_x + i\psi_y & -\psi_z & 0 & 0 \\ 0 & 0 & \psi_z & \psi_x - i\psi_y \\ 0 & 0 & \psi_x + i\psi_y & -\psi_z \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} a' \\ b' \\ c' \\ d' \end{pmatrix}$$

and we can form a similar matrix that includes σ, τ, and $\sigma\tau$ operators.

Propagation of spinors

Here is how the matrix for rotations of spins is calculated:

```
stmat(1,1)=rots(3)
stmat(1,2)=rots(1)-ci*rots(2)
stmat(2,1)=rots(1)+ci*rots(2)
stmat(2,2)=-rots(3)
stmat(3,3)=rots(3)
stmat(3,4)=rots(1)-ci*rots(2)
stmat(4,3)=rots(1)+ci*rots(2)
stmat(4,4)=-rots(3)
```

$$\begin{pmatrix} \psi_z & \psi_x - i\psi_y & 0 & 0 \\ \psi_x + i\psi_y & -\psi_z & 0 & 0 \\ 0 & 0 & \psi_z & \psi_x - i\psi_y \\ 0 & 0 & \psi_x + i\psi_y & -\psi_z \end{pmatrix}$$

Propagation of spinors

The full matrix with σ, τ, and $\sigma\tau$:

```
stmat(1,1)=rots(3)+rott(3)+rotst(3,3)
stmat(1,2)=rots(1)-ci*rots(2)+rotst(1,3)-ci*rotst(2,3)
stmat(1,3)=rott(1)-ci*rott(2)+rotst(3,1)-ci*rotst(3,2)
stmat(1,4)=rotst(1,1)-ci*rotst(2,1)-ci*rotst(1,2)-rotst(2,2)
stmat(2,1)=rots(1)+ci*rots(2)+rotst(1,3)+ci*rotst(2,3)
stmat(2,2)=-rots(3)+rott(3)-rotst(3,3)
stmat(2,3)=rotst(1,1)-ci*rotst(1,2)+ci*rotst(2,1)+rotst(2,2)
stmat(2,4)=rott(1)-ci*rott(2)-rotst(3,1)+ci*rotst(3,2)
stmat(3,1)=rott(1)+ci*rott(2)+rotst(3,1)+ci*rotst(3,2)
stmat(3,2)=rotst(1,1)+ci*rotst(1,2)-ci*rotst(2,1)+rotst(2,2)
stmat(3,3)=rots(3)-rott(3)-rotst(3,3)
stmat(3,4)=rots(1)-ci*rots(2)-rotst(1,3)+ci*rotst(2,3)
stmat(4,1)=rotst(1,1)+ci*rotst(2,1)+ci*rotst(1,2)-rotst(2,2)
stmat(4,2)=rott(1)+ci*rott(2)-rotst(3,1)-ci*rotst(3,2)
stmat(4,3)=rots(1)+ci*rots(2)-rotst(1,3)-ci*rotst(2,3)
stmat(4,4)=-rots(3)-rott(3)+rotst(3,3)
```

Propagation of spinors

Then, the last operation to do is to use the previous matrix to rotate spinors:

$$e^M|s_n\rangle = |s_n'\rangle$$

and one easy way is to expand the exponent (remember that $|s_n\rangle$ is a vector):

$$e^M|s_n\rangle \approx |s_n + Ms_n + \frac{1}{2}M\,Ms_n + \ldots\rangle = |s_n'\rangle$$

Is this expansion accurate? YES! Remember that the M matrix contains the time-step $\delta\tau$ that is small!

Auxiliary Field Diffusion Monte Carlo

Many other details needed, but overall these slides summarize the difference between AFDMC and the regular DMC.

More details in the afternoon.

Auxiliary Field Diffusion Monte Carlo

Many other details needed, but overall these slides summarize the difference between AFDMC and the regular DMC.

More details in the afternoon.