Auxiliary Field Diffusion Monte Carlo

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Spin-dependent interactions

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Let's define a spinor for each nucleon (in addition to the spacial coordinate $\vec{r}$):

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

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:

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

Spin-dependent interactions

Unless specified, let's just consider the spin or particles, (the addition of the isospin is trivial). Suppose that we want to use a simpler wave function with the "simple" structure given by the product of single particle spinors, i.e.

$$\langle S|\Psi\rangle \propto \xi_{\alpha_1}(s_1)\xi_{\alpha_2}(s_2)\dots\xi_{\alpha_N}(s_N)$$

where $\xi_{\alpha_i}(s)$ are functions of the spinor s with state α_i (more details later), and $S = \{s_1 \dots s_N\}$.

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This (easy) form requires N^3 (vs 2^N) operations to be computed. However it cannot be used for quadratic spin/isospin operators because:

$$\sigma \cdot \sigma|\Psi\rangle \propto |\Psi'\rangle + |\Psi''\rangle$$

Spin-dependent interactions

Example:

$$\langle S|\Psi\rangle = \xi_{\alpha_1}(s_1)\xi_{\alpha_2}(s_2)\xi_{\alpha_3}(s_3)$$

then

$$\begin{aligned}\langle S|\sigma_1\cdot\sigma_2|\Psi\rangle &= \langle S|2P_{12}^{\sigma}-1|\Psi\rangle = \\ &= 2\xi_{\alpha_1}(s_2)\xi_{\alpha_2}(s_1)\xi_{\alpha_3}(s_3) - \xi_{\alpha_1}(s_1)\xi_{\alpha_2}(s_2)\xi_{\alpha_3}(s_3) = \\ &= \langle S|\Psi'\rangle + \langle S|\Psi''\rangle\end{aligned}$$

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Thus a propagator like $\sum_{i,j}\sigma_i\cdot\sigma_j$ acting on a wave function of this type generates many many different amplitudes.

Suppose that we have instead a linear operator:

$$\begin{aligned}\langle S|\sigma_1^{\alpha}|\Psi\rangle &= \sigma_1^{\alpha}\xi_{\alpha_1}(s_1)\xi_{\alpha_2}(s_2)\xi_{\alpha_3}(s_3) = \\ &= \xi_{\alpha_1}(s_1')\xi_{\alpha_2}(s_2)\xi_{\alpha_3}(s_3) = \langle S|\Psi'\rangle\end{aligned}$$

This is fine!

Hubbard-Stratonovich transformation

How do we *linearize* quadratic operators?

Remember that we have in the propagator something like:

$$e^{-\sum_{i<j} v(r_{ij}) \sigma_i \cdot \sigma_j \delta\tau}$$

Hubbard-Stratonovich transformation:

$$e^{-\frac{1}{2}\lambda \hat{O}^2} = \frac{1}{\sqrt{2\pi}} \int dx \, e^{-\frac{x^2}{2} + \sqrt{-\lambda} x \hat{O}}$$

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The Hubbard-Stratonovich transformation is exact when the integral(s) are properly solved. And they can be solved using Monte Carlo!

$$\frac{1}{\sqrt{2\pi}} \int dx \, e^{-\frac{x^2}{2} + \sqrt{-\lambda} x \hat{O}} = \frac{1}{\sqrt{2\pi}} \int dx \, P(x) \, e^{\sqrt{-\lambda} x \hat{O}}$$

Hubbard-Stratonovich transformation

Let's consider as an example the free Hamiltonian:

$$\exp\left[-\sum_n \frac{\mathbf{p}_n^2}{2m}\delta\tau\right] \approx \prod_n \exp\left(-\frac{\mathbf{p}_n^2}{2m}\delta\tau\right)$$
$$= \prod_n \frac{1}{(2\pi)^{3/2}} \int dx_n e^{-x_n^2/2} \exp\left(-\frac{i}{\hbar}\mathbf{p}_n x_n \sqrt{\frac{\hbar^2\delta\tau}{m}}\right)$$

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This propagator applied to a walker $|\mathbf{R}\rangle$ generates a new position $|\mathbf{R}+\Delta\mathbf{R}\rangle$, where each particle position is shifted as

$$\mathbf{r}'_n = \mathbf{r}_n + \frac{\hbar^2\delta\tau}{m} x_n \,.$$

This is identical to the standard diffusion Monte Carlo algorithm without importance sampling. Each particle is moved with a Gaussian distribution of variance $\hbar^2\delta\tau/m$, and a weight of $\exp[E_T)\delta\tau]$ is included. The branching on the weight is then included to complete the algorithm.

Nucleon-nucleon interaction

Let's consider a v_6 form of nucleon-nucleon interactions for neutrons ($\tau \cdot \tau = 1$):

$$
\begin{aligned}
v_6(ij) &= v_c(r_{ij}) + v_\tau(r_{ij}) + [v_\sigma(r_{ij}) + v_{\sigma\tau}]\,\sigma_i \cdot \sigma_j + [v_t(r_{ij}) + v_{t\tau}(r_{ij})]\,S_{ij} \\
&= V_{SI} + (v_\sigma + v_{\sigma\tau})\sigma_i \cdot \sigma_j + (v_t + v_{t\tau})(3\sigma_i \cdot \hat{r}_{ij} \cdot \sigma_j \hat{r}_{ij} - \sigma_i \cdot \sigma_j) \\
&= V_{SI} + \sum_{\alpha\beta}[(v_\sigma + v_{\sigma\tau})\sigma_i^\alpha \sigma_j^\beta \delta_{\alpha\beta} + (v_t + v_{t\tau})(3\sigma_i^\alpha \hat{r}_{ij}^\alpha \sigma_j^\beta \hat{r}_{ij}^\beta - \sigma_i^\alpha \sigma_j^\beta \delta_\alpha\beta)] \\
&= V_{SI} + \sum_{\alpha\beta} \sigma_i^\alpha [(v_\sigma + v_{\sigma\tau} - v_t - v_{t\tau})\delta_{\alpha\beta} + 3(v_t + v_{t\tau})\hat{r}_{ij}^\alpha \hat{r}_{ij}^\beta]\sigma_j^\beta \\
&= V_{SI} + \sum_{\alpha\beta} \sigma_i^\alpha A_{i\alpha j\beta} \sigma_j^\beta
\end{aligned}
$$

where V_{SI} is the spin-independent part of the interaction, and the matrix A contains all (and just) the radial dependence of the interaction.

Nucleon-nucleon interaction

Quadratic spin- isospin-dependent interactions can be written in the form:

$$V = \sum_{i<j} v(ij) = \frac{1}{2} \sum_{ij} S_i A_{ij} S_j$$

where A is real and symmetric, and can be diagonalized:

$$\sum_j A_{ij} \psi_j^{(n)} = \lambda_n \psi_i^{(n)}$$

Then

$$A_{ij} = \sum_n \psi_i^{(n)} \lambda_n \psi_j^{(n)}$$

and finally

$$V = \frac{1}{2} \sum_{i,j} \sum_{\alpha\beta} \sigma_i^\alpha A_{i\alpha j\beta} \sigma_j^\beta = \frac{1}{2} \sum_n \lambda_n O_n^2 , \qquad O_n = \sum_j \psi_j^{(n)} S_j$$

A first easy example

Let's consider two neutrons. The propagator (just for the interaction) is:

$$\exp\left[-v(r)\vec{\sigma}_1 \cdot \vec{\sigma}_2 \delta\tau\right]$$

We can use:

$$\vec{\sigma}_1 \cdot \vec{\sigma}_2 = \frac{(\vec{\sigma}_1 + \vec{\sigma}_2)^2 - \vec{\sigma}_1^2 - \vec{\sigma}_2^2}{2}$$

and then:

$$\exp\left[-v(r)\vec{\sigma}_1 \cdot \vec{\sigma}_2 \delta\tau\right] = \exp\left[-v(r)\frac{(\vec{\sigma}_1 + \vec{\sigma}_2)^2 - \vec{\sigma}_1^2 - \vec{\sigma}_2^2}{2}\delta\tau\right]$$

and use the Hubbard Stratonovich for the quadratic parts!

Nucleon-nucleon interaction

In summary: for the interaction, we need to construct three matrices $A^{(\sigma)}$, $A^{(\tau)}$ and $A^{(\sigma\tau)}$, diagonalize them, and then calculate the corresponding operators $O_n^{(\sigma)}$, $O_n^{(\tau)}$ and $O_n^{(\sigma\tau)}$.

The interaction is the rewritten as

$$V_{SD} = \frac{1}{2}\sum_{n=1}^{3A} O_n^{(\sigma)2}\lambda_n^{(\sigma)} + \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{3A} O_{n\alpha}^{(\sigma\tau)2}\lambda_n^{(\sigma\tau)} + \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{A} O_{n\alpha}^{(\tau)2}\lambda_n^{(\tau)}$$

Nucleon-nucleon interaction

The full propagator (without importance sampling) is then rewritten as:

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

Note: to sample the interaction we need 15 operators for each nucleon, 3 σ, 3 τ, and 9 $\sigma\tau$.

Spinor propagation

Let's see how to propagate the spinor of the n-th nucleon for a given (sampled) auxiliary field x_n:

$$
\begin{aligned}
& e^{\sqrt{-\lambda_n \delta\tau} x_n O_n} \left| s_n \right\rangle = \\
& = e^{\sqrt{-\lambda_n \delta\tau} x_n \sum_\alpha \sum_{j\beta} \tau_{j\alpha} \sigma_{j\beta} \psi^{(n)}_{j\beta}} \left| s_n \right\rangle = \\
& = e^M \left| s_n \right\rangle = \left| s'_n \right\rangle
\end{aligned}
$$

where M is a 4×4 matrix that depends upon $\psi_{j\beta}$ and the operators τ_α and σ_β.

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\end{aligned}
$$

where M is a 4×4 matrix that depends upon $\psi_{j\beta}$ and the operators τ_α and σ_β. Example: matrix to rotate the spin part (the sum over j is understood)

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

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):

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

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

Auxiliary Field Diffusion Monte Carlo

The idea of Auxiliary Field Diffusion Monte Carlo (AFDMC) is to propagate coordinates on the continuum as commonly done in Diffusion Monte Carlo. The spin states of nucleons are also sampled on the continuum using auxiliary fields.

AFDMC wave function

Let's just consider the spin of nucleons. The trial (variational) wave function 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.

In this example, 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

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

AFDMC wave function

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

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

Auxiliary Field Diffusion Monte Carlo

The AFDMC algorithm can be summarized in the following steps:

1. Generate a set of N walkers randomly or distributed with VMC
2. Loop over the N walkers, and for each walker:
3. Generate a Gaussian step ΔR and Gaussian auxiliary fields X
4. Move particles' positions (to propagate the kinetic energy)
5. Rotate particles' spinors (to propagate the potential energy)
6. Calculate the weight (including E_T and V_{SI})
7. Do branching
8. Increase the total imaginary-time by a unit of $\delta\tau$
9. Iterate with 2) until the equilibration is reached, then reset estimators and iterate until the error is small enough

Auxiliary Field Diffusion Monte Carlo

Other caveats:

- Trial wave function now is spin- and isospin-dependent, can also contains (simple) spin- isospin-dependent correlations
- Sign problem (constrained path), but unconstrained-path possible
- Spin-orbit and three-body interactions more difficult (but possible) to include
- AFDMC moderately expensive, used so far up to $\sim$100 nucleons!
- Used for nuclei, nuclear and neutron matter, confined neutrons, ...
- Very active field with continuous developments! Interested?

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