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.

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

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

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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 propagators 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

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

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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?

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 a first case a scalar Hamiltonian:

$$\exp\left[-V(R)\delta\tau - \sum_n \frac{\mathbf{p}_n^2}{2m}\delta\tau\right] \approx \exp\left[-V(R)\delta\tau\right]\prod_n \exp\left(-\frac{\mathbf{p}_n^2}{2m}\delta\tau\right)$$

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

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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 $\exp[-(V(\mathbf{R})-E_T)\delta\tau]$ is included. The branching on the weight is then included to complete the algorithm.

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

$$V = \frac{1}{2}\sum_{ij} S_i A_{ij} S_j$$

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

$$V = \frac{1}{2}\sum_n \lambda_n O_n^2 \,, \qquad O_n = \sum_j \psi_j^{(n)} S_j$$

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

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.

Nucleon-nucleon interaction

Now we can diagonalize $A_{i\alpha j\beta}$:

$$\sum_{j\beta} A_{i\alpha j\beta}\psi^{(n)}_{j\beta} = \lambda_n \psi^{(n)}_{i\alpha}$$

and define new operators

$$O_n = \sum_{j\beta} \sigma_{j\beta}\psi^{(n)}_{j\beta}$$

such that

$$V_{SD} = \frac{1}{2}\sum_{\alpha}\sum_{n} O^2_{n\alpha}\lambda_n$$

Exercise: extend to include the isospin

Nucleon-nucleon interaction

For the full v_4 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: for the v_4 and v_6 interaction there are 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}|s_n\rangle = \\
& = e^{\sqrt{-\lambda_n\delta\tau}x_n \sum_\alpha \sum_{j\beta} \tau_{j\alpha}\sigma_{j\beta}\psi^{(n)}_{j\beta}}|s_n\rangle = \\
& = e^M|s_n\rangle = |s'_n\rangle
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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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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)

$$
\left(\begin{array}{cccc}
\psi_z & \psi_x - i\psi_y & 0 & 0 \\
\psi_x + i\psi_y & -\psi_z & 0 & 0 \\
0 & 0 & \psi_z & \psi_x - i\psi_y \\
0 & 0 & \psi_x + i\psi_y & -\psi_z
\end{array} \right)
\left(\begin{array}{c} a \\ b \\ c \\ d \end{array} \right)
=
\left(\begin{array}{c} a' \\ b' \\ c' \\ d' \end{array} \right)
$$

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.

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Don't confuse with Auxiliary Field Monte Carlo, Auxiliary Field Quantum Monte Carlo, etc., commonly used for condensed matter and also in nuclear physics!

Dean and Joaquin will talk about other methods using auxiliary fields next weeks!

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. Sample one move from $(\Delta R, X)$, $(\Delta R, -X)$, $(-\Delta R, X)$ and $(-\Delta R, -X)$, shifting particles by ΔR (and $-\Delta R$) and rotating spinors using X (and $-X$).
5. Calculate the weight
6. Do branching
7. Increase the total imaginary-time by a unit of $\delta\tau$
8. 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?

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... for now :-)