

Dissertation Defense:
Improved Trial Wave Functions for Quantum
Monte Carlo Calculations of Nuclear Systems and
Their Applications

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Outline

1 Motivation

2 Research

- QMC Methods
- Trial Wave Function
- Alpha Formation in NS

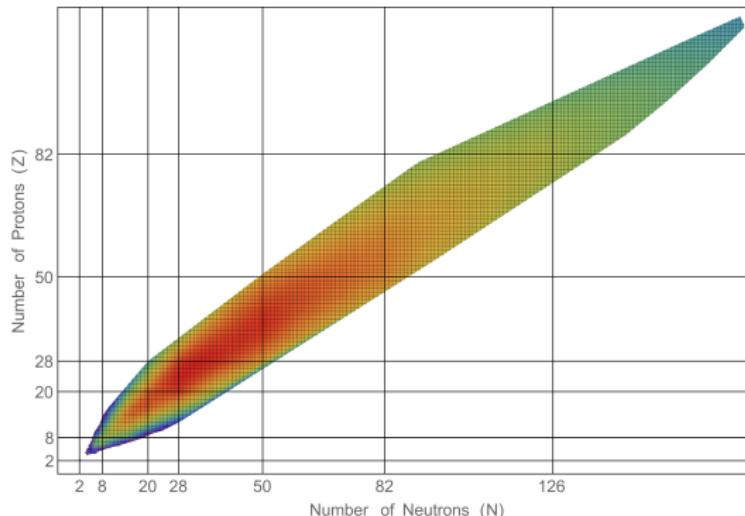
3 Conclusion

- Future Work
- Conclusion

Nuclear Many Body Problem

$$\langle H \rangle = \langle \Psi | H | \Psi \rangle = \int \Psi^*(\mathbf{R}) H \Psi(\mathbf{R}) d\mathbf{R}$$

$$H = \sum_{i=1}^A \frac{\mathbf{p}_i^2}{2m} + \sum_{i < j} v_{ij} + \sum_{i < j < k} V_{ijk} + \dots$$



Nuclear Many Body Methods

- There are a number of ways to solve this problem.
 - Hartree-Fock
 - Basis-set methods
 - No-core shell model
 - Coupled-cluster
 - Self consistent Green's function method
 - Quantum Monte Carlo
 - VMC
 - GFMC
 - AFDMC

Variational Monte Carlo

- VMC starts with a trial wave function which includes variable parameters.
- Variational energy is an upper bound to the ground state energy.

$$E_V = \frac{\int \psi_T^*(\mathbf{R}) H \psi_T(\mathbf{R}) d\mathbf{R}}{\int \psi_T^*(\mathbf{R}) \psi_T(\mathbf{R}) d\mathbf{R}} \geq E_0$$

- Integral is solved with MC integration.

$$E_V = \int f(\mathbf{R}) P(\mathbf{R}) d\mathbf{R} \approx \frac{1}{N} \sum_{n=1}^N f(\mathbf{R}_n)$$

Variational Monte Carlo

$$E_V = \int P(\mathbf{R}) E_L(\mathbf{R}) d\mathbf{R}$$

- Multiply and divide the numerator by $\Psi_T^*(\mathbf{R})\Psi_T(\mathbf{R})$.

$$P(\mathbf{R}) = \frac{|\Psi_T(\mathbf{R})|^2}{\int |\Psi_T(\mathbf{R})|^2 d\mathbf{R}}, \quad E_L(\mathbf{R}) = \frac{\Psi_T^*(\mathbf{R}) H \Psi_T(\mathbf{R})}{\Psi_T^*(\mathbf{R}) \Psi_T(\mathbf{R})}$$

- Now using Monte Carlo integration we can write

$$E_V \approx \frac{1}{N} \sum_{n=1}^N E_L(\mathbf{R}_n),$$

where the \mathbf{R}_n are samples from $P(\mathbf{R})$.

Variational Monte Carlo

- The statistical error in the energy is then given in the typical way

$$\sigma_{E_V} = \sqrt{\frac{\langle E_L^2 \rangle - \langle E_L \rangle^2}{N}} \approx \sqrt{\frac{\left(\frac{1}{N} \sum_{n=1}^N E_L^2(\mathbf{R}_n) \right) - \left(\frac{1}{N} \sum_{n=1}^N E_L(\mathbf{R}_n) \right)^2}{N-1}}$$

- We can then vary the parameters in the trial wave function and calculate this until we minimize the energy or statistical error, since $E_V \geq E_0$.

Diffusion Monte Carlo

- Diffusion Monte Carlo uses a Green's function to diffuse in imaginary time to estimate the ground state energy and wave function based on a trial wave function.

$$H\Psi = i\hbar \frac{d\Psi}{dt} \xrightarrow{\tau=it/\hbar} H\Psi = -\frac{d\Psi}{d\tau}$$

Using separation of variables we can write

$$\Psi(\mathbf{R}, \tau) = \sum_{n=0}^{\infty} c_n \phi_n(\mathbf{R}) e^{-\tau(E_n - E_0)}$$

- The long imaginary time limit of this goes to the ground state.

$$\lim_{\tau \rightarrow \infty} \Psi(\mathbf{R}, \tau) = c_0 \phi_0(\mathbf{R})$$

Diffusion Monte Carlo

- The propagated wave function can be written

$$\langle \mathbf{R}' | \Psi_T(\tau) \rangle = \int d\mathbf{R} \langle \mathbf{R}' | e^{-(H-E_0)\tau} | \mathbf{R} \rangle \langle \mathbf{R} | \Psi_T(0) \rangle$$

- Now we use $e^{-H\tau} = e^{-V\tau/2}e^{-T\tau}e^{-V\tau/2} + \mathcal{O}(\tau^3)$ and break up the propagator into small time steps $\Delta\tau = \tau/N$.

$$\langle \mathbf{R}_N | \Psi_T(\tau) \rangle = \int d\mathbf{R}_1 \dots d\mathbf{R}_N \left[\prod_{i=1}^N G(\mathbf{R}_i, \mathbf{R}_{i-1}, \Delta\tau) \right] \langle \mathbf{R}_0 | \Psi_T(0) \rangle$$

$$G(\mathbf{R}', \mathbf{R}, \Delta\tau) = \langle \mathbf{R}' | e^{-(H-E_0)\Delta\tau} | \mathbf{R} \rangle$$

Diffusion Monte Carlo

- In the small $\Delta\tau$ limit this propagator can be split up with the kinetic term being used to diffuse the walkers along a random path.

$$\langle \mathbf{R}' | e^{-T\Delta\tau} | \mathbf{R} \rangle = \left(\frac{m}{2\pi\hbar^2\Delta\tau} \right)^{3A/2} e^{-m(\mathbf{R}' - \mathbf{R})^2/2\hbar^2\Delta\tau}$$

- The potential term can then be used as a weight in a branching algorithm.

$$w(\mathbf{R}') = e^{-(V(\mathbf{R}') + V(\mathbf{R}) - 2E_0)\Delta\tau/2}$$

- Importance sampling improves the variance of the sampling and can be included with

$$G(\mathbf{R}', \mathbf{R}, \Delta\tau) \rightarrow G(\mathbf{R}', \mathbf{R}, \Delta\tau) \frac{\langle \mathbf{R} | \Psi_I \rangle}{\langle \mathbf{R}' | \Psi_I \rangle}$$

Diffusion Monte Carlo - Branching

Branching: Each walker can be deleted or multiply. The number of walkers that continues is equal to $\text{int}(w(\mathbf{R}') + \xi)$, where ξ is a uniform random number from $[0, 1]$.

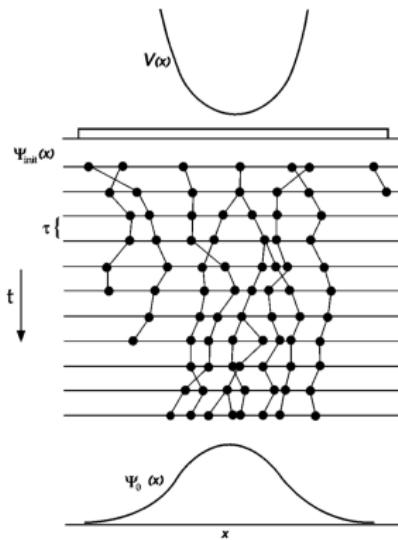


Figure: Reprinted from W.M.C. Foulkes et al.
Rev. Mod. Phys., 73:33-83, 2001.

Estimating Expectation Values

We want to solve something like this

$$\langle \mathcal{O} \rangle = \frac{\langle \Psi(\tau) | \mathcal{O} | \Psi(\tau) \rangle}{\langle \Psi(\tau) | \Psi(\tau) \rangle}.$$

In practice a linear extrapolation is used because $\mathcal{O}\Psi(\tau)$ is hard.

$$\langle \mathcal{O} \rangle \approx 2 \langle \mathcal{O} \rangle_{\text{mixed}} - \langle \mathcal{O} \rangle_{\text{VMC}}$$

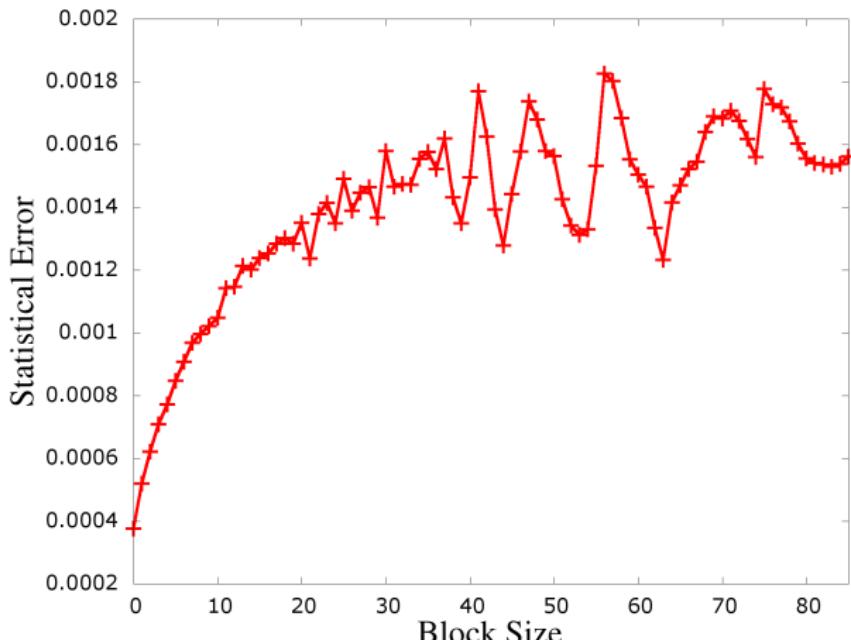
$$\langle \mathcal{O} \rangle_{\text{mixed}} = \frac{\langle \Psi(\tau) | \mathcal{O} | \Psi_T \rangle}{\langle \Psi(\tau) | \Psi_T \rangle}, \quad \langle \mathcal{O} \rangle_{\text{VMC}} = \frac{\langle \Psi_T | \mathcal{O} | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$$

In the large τ limit when $[\mathcal{O}, H] = 0$

$$\lim_{\tau \rightarrow \infty} \langle \mathcal{O} \rangle_{\text{mixed}} = \langle \mathcal{O} \rangle$$

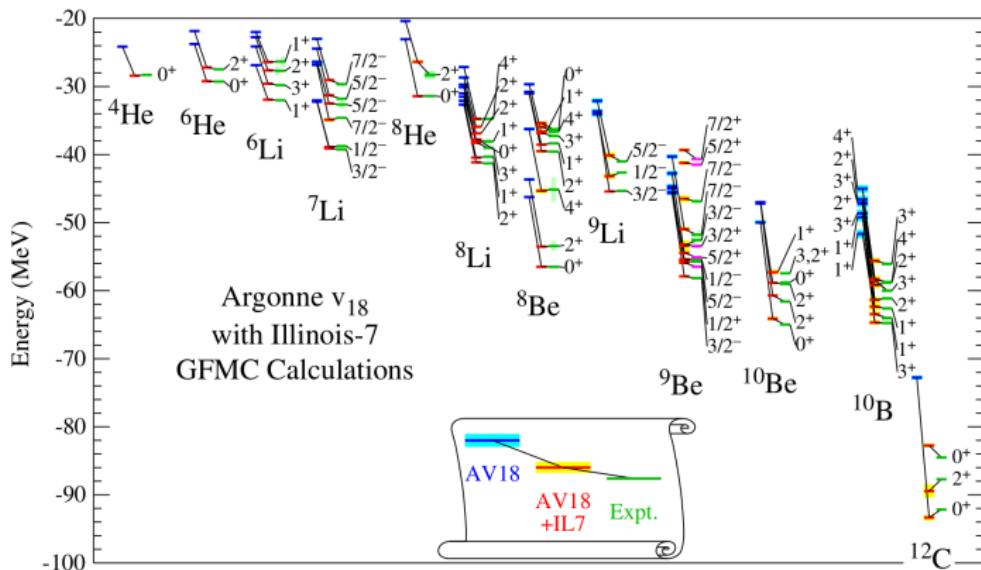
Estimating Error

Our energy estimates are correlated and so we estimate error using block averaging



Green's Function Monte Carlo

- GFMC follows DMC exactly for the spatial integrals, but performs the sums of 2^A spin and $\frac{A!}{Z!(A-Z)!}$ isospin states, for A nucleons with Z protons explicitly.



Auxiliary Field Diffusion Monte Carlo - Spin Sampling

- Mimicking the diffusion in DMC, AFDMC samples auxiliary fields to rotate the spins/isospins of the walkers.
- The spin-isospin dependent part of the potential is what is used in the spin-isospin dependent part of the propagator.

$$G_{SD}(R'S', RS, \Delta\tau) = \langle R'S' | e^{-V_{SD}\Delta\tau} | RS \rangle$$

$$V_{SD} = \sum_{p=2}^6 \sum_{i < j} v_p(r_{ij}) \mathcal{O}_{ij}^p$$

- For v_6 , a truncation of the phenomenological Argonne v_{18} potential, the operators are $\sigma_i \cdot \sigma_j$, $\tau_i \cdot \tau_j$, $\sigma_i \cdot \sigma_j \tau_i \cdot \tau_j$, S_{ij} and $S_{ij} \tau_i \cdot \tau_j$, where $S_{ij} = 3\sigma_i \cdot \hat{r}_{ij} \sigma_j \cdot \hat{r}_{ij} - \sigma_i \cdot \sigma_j$

Auxiliary Field Diffusion Monte Carlo - Spin Sampling

- The spin-isospin dependent operators

$$\begin{aligned} G_{SD}(R'S', RS, \Delta\tau) &= \langle R'S' | e^{-V_{SD}\Delta\tau} | RS \rangle \\ &= \langle R'S' | e^{-\sum_{p=2}^6 \sum_{i < j} v_p(r_{ij}) \mathcal{O}_{ij}^p \Delta\tau} | RS \rangle \end{aligned}$$

is sampled by using the Hubbard-Stratanovich transformation.

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

Auxiliary Field Diffusion Monte Carlo - Spin Sampling

- The potential can be written in terms of matrices that are made of the $v_p(r_{ij})$, are symmetric, and 0 if $i = j$.

$$V_{SD} = \frac{1}{2} \sum_{i\alpha j\beta} \sigma_{i\alpha} A_{i\alpha j\beta}^\sigma \sigma_{j\beta} + \frac{1}{2} \sum_{i\alpha j\beta} \sigma_{i\alpha} A_{i\alpha j\beta}^{\sigma\tau} \sigma_{j\beta} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j + \frac{1}{2} \sum_{ij} A_{ij}^\tau \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$$

- We can construct these matrices and then solve for their eigenvalues and eigenvectors.

$$\sum_{j\beta} A_{i\alpha j\beta}^\sigma \psi_{nj\beta}^\sigma = \lambda_n^\sigma \psi_{ni\alpha}^\sigma$$

$$\sum_{j\beta} A_{i\alpha j\beta}^{\sigma\tau} \psi_{nj\beta}^{\sigma\tau} = \lambda_n^{\sigma\tau} \psi_{ni\alpha}^{\sigma\tau}$$

$$\sum_j A_{ij}^\tau \psi_{nj}^\tau = \lambda_n^\tau \psi_{ni}^\tau$$

Auxiliary Field Diffusion Monte Carlo - Spin Sampling

- The potential can then be written in terms of the square of new single particle operators.

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

$$O_n^\sigma = \sum_{j\beta} \sigma_{j\beta} \psi_{nj\beta}^\sigma$$

$$O_{n\alpha}^{\sigma\tau} = \sum_{j\beta} \tau_{j\alpha} \sigma_{j\beta} \psi_{nj\beta}^{\sigma\tau}$$

$$O_{n\alpha}^\tau = \sum_j \tau_{j\alpha} \psi_{nj}^\tau$$

Auxiliary Field Diffusion Monte Carlo - Spin Sampling

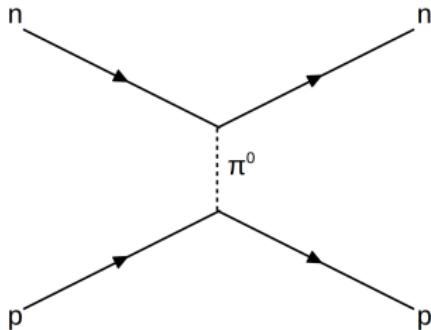
- We have squared single particle operators in the propagator we can now rewrite the propagator in terms of the Hubbard-Stratanovich transformation.

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

- We have 15A operators (3A for O_n^σ , 9A for $O_{n\alpha}^{\sigma\tau}$, and 3A for $O_{n\alpha}^\tau$), the spin-isospin dependent part of the propagator becomes

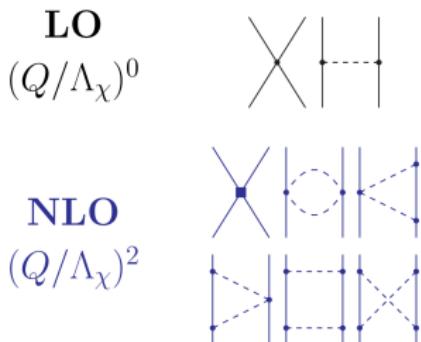
$$G_{SD}(R'S', RS, \Delta\tau) = \prod_{n=1}^{15A} \frac{1}{\sqrt{2\pi}} \int dx_n e^{-\frac{x_n^2}{2}} e^{\sqrt{-\lambda_n \Delta\tau} x_n O_n}.$$

Hamiltonian



Based on meson exchange

- Argonne v_{18} (NN)
- CD-Bonn (NN)
- Urbana UIX (NNN)
- Illinois (NNN)



Based on χ EFT expansion in momentum (up to N²LO)

Figure from R. Machleidt and D.R. Entem, *Chiral effective field theory and nuclear forces*, Phys. Rep. 503, 1 (2011)

Hamiltonian - Argonne v6' (AV6')

- For this work I have used the NN AV6' potential with no 3N interaction, though I will be showing some preliminary results with the χ EFT NN and 3N potentials up to N²LO.
- First 6 operators of the AV18 potential

$$v_{ij} = \sum_{p=1}^6 v_p(\mathbf{r}_{ij}) \mathcal{O}_{ij}^p$$

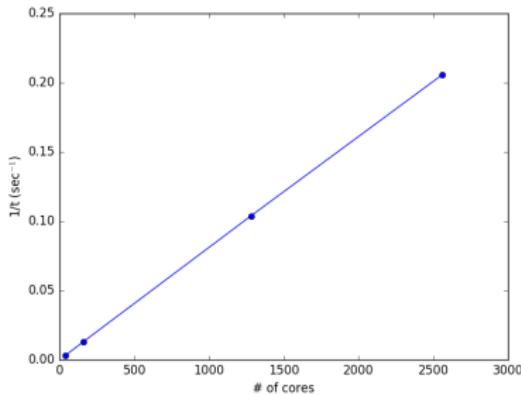
$$\mathcal{O}_{ij}^p = 1, \ \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j, \ \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, \ \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j, \ S_{ij}, \ S_{ij} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$$

$$S_{ij} = 3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$$

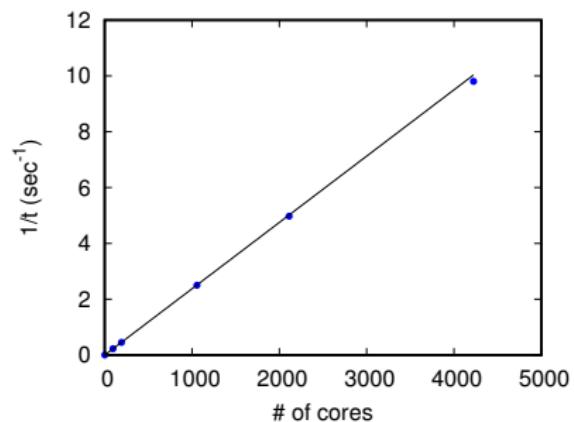
Scaling

- We have written our own AFDMC code.
- Not currently open source, but should be soon.
- Run on CPU made available through XSEDE allocations.

Time to propagate 10,000 walkers of ^{16}O for 100 steps.



SuperMIC (LSU)



Stampede 2 (TACC)

Trial Wave Function - Slater Determinant

- Properties:
 - Antisymmetric
 - Cluster Decomposable
$$|A + B\rangle = |A\rangle |B\rangle$$

- The simplest wave function for a many-fermion system obeying these properties is a Slater determinant where $\phi_i(\mathbf{r}_i, s_i)$ are single particle nucleon states.

$$\psi_T = \langle RS|\phi\rangle = \mathcal{A} \prod_{i=1}^A \phi_i(\mathbf{r}_i, s_i) = \frac{1}{A!} \det \phi_k(\mathbf{r}_I, s_I)$$

- Short range correlations need to be put in by hand via Jastrow-like correlations.

$$|\psi_T\rangle = \prod_{i < j} f(r_{ij}) |\phi\rangle .$$

Spin Dependent Correlations

- Two spin dependent wave functions that obey these two properties are the exponentially correlated and symmetrized product wave functions, where \mathcal{O}_{ij}^P are the AV6 operators, $\sigma_i \cdot \sigma_j$, $\tau_i \cdot \tau_j$, $\sigma_i \cdot \sigma_j \tau_i \cdot \tau_j$, S_{ij} and $S_{ij} \tau_i \cdot \tau_j$, where $S_{ij} = 3\sigma_i \cdot \hat{r}_{ij} \sigma_j \cdot \hat{r}_{ij} - \sigma_i \cdot \sigma_j$.

$$|\psi_T\rangle = \left[\prod_{i < j} f_c(r_{ij}) \right] e^{\sum_{i < j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^P} |\phi\rangle$$

$$|\psi_T\rangle = \left[\prod_{i < j} f_c(r_{ij}) \right] S \prod_{i < j} \left(1 + \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^P \right) |\phi\rangle$$

- These two wave functions are the same up to second order except for commutator terms.

Expand to Linear Correlations

- Because of the cost for larger systems in 2007 they only included Jastrow correlations.

$$|\psi_T\rangle = \left[\prod_{i < j} f_c(r_{ij}) \right] |\phi\rangle$$

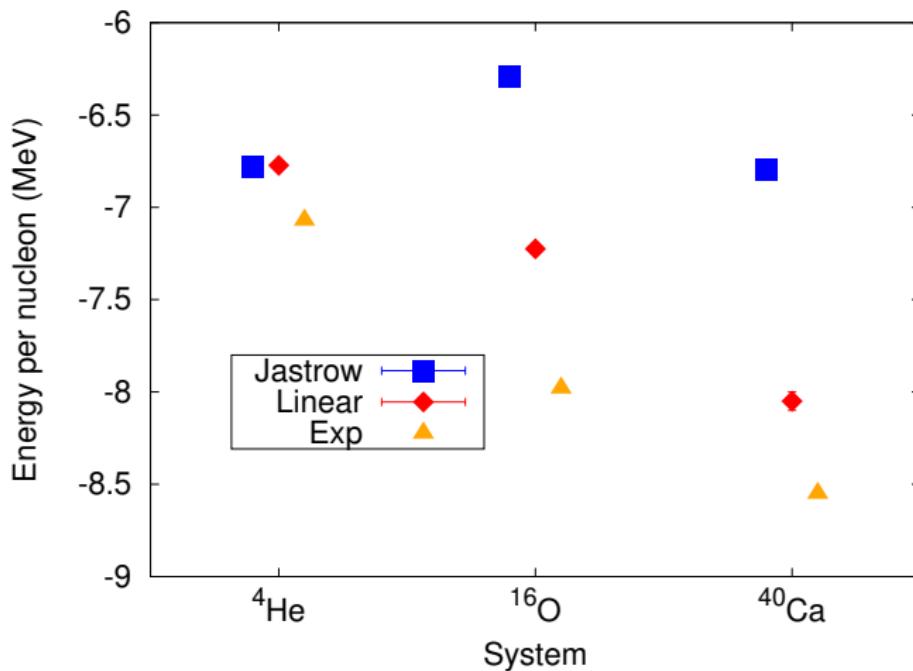
S. Gandolfi et al. *Phys. Rev. Lett.*, **99**, 022507, 2007.

- By 2014 they added spin-isospin correlations to improve overlap with tensor. This is a truncated expansion of either full wave function from before.

$$|\psi_T\rangle = \left[\prod_{i < j} f_c(r_{ij}) \right] \left(1 + \sum_{i < j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p \right) |\phi\rangle$$

S. Gandolfi et al. *Phys. Rev. C.*, **90**, 061306(R), 2014.

Compare Jastrow to Jastrow+Linear

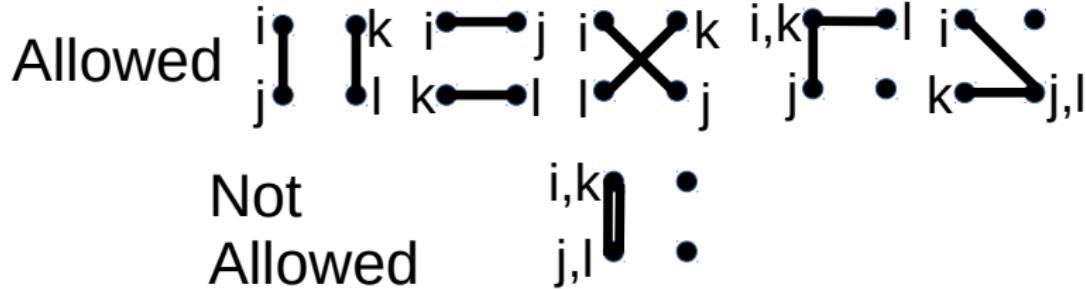


Data taken from each paper respectively.

Symmetrized Product Wave Function

- The logical next step was to keep more terms in the expansion.

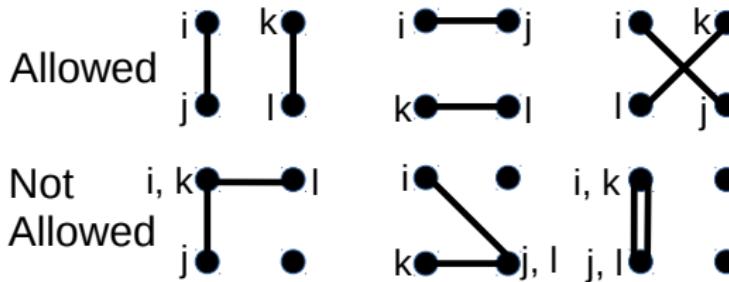
$$\begin{aligned} |\psi_T\rangle = & \left[\prod_{i < j} f_c(r_{ij}) \right] \left[1 + \sum_{i < j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p \right. \\ & \left. + \frac{1}{2} \sum_{i < j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p \sum_{\substack{k < l \\ ij \neq kl}} \sum_q f_q(r_{kl}) \mathcal{O}_{kl}^q \right] |\phi\rangle \end{aligned}$$



Independent Pair Quadratic Correlations

- Or it can be expanded to get independent pair quadratic terms

$$|\psi_T\rangle = \left[\prod_{i < j} f_c(r_{ij}) \right] \left[1 + \sum_{i < j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p + \sum_{i < j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p \sum_{k < l, ip} f_q(r_{kl}) \mathcal{O}_{kl}^q \right] |\phi\rangle$$



Quadratic Correlations Implementation

- Much of my work was in working out the math and programming for implementing these correlations in an efficient way into the VMC and AFDMC code.
- More details of their implementation can be found in my dissertation, I will be focusing on the physical results.

Results - AFDMC

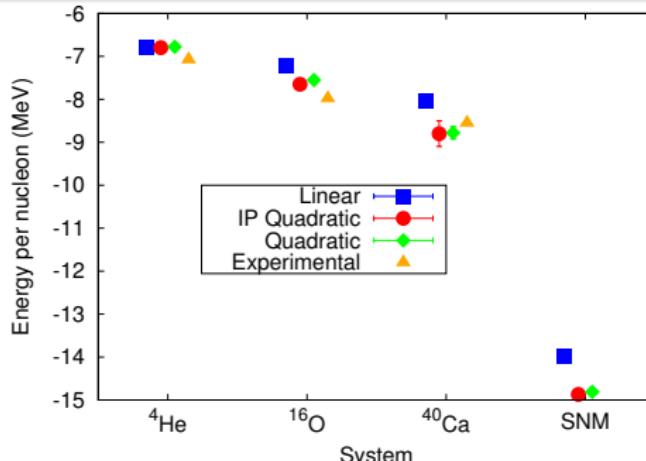
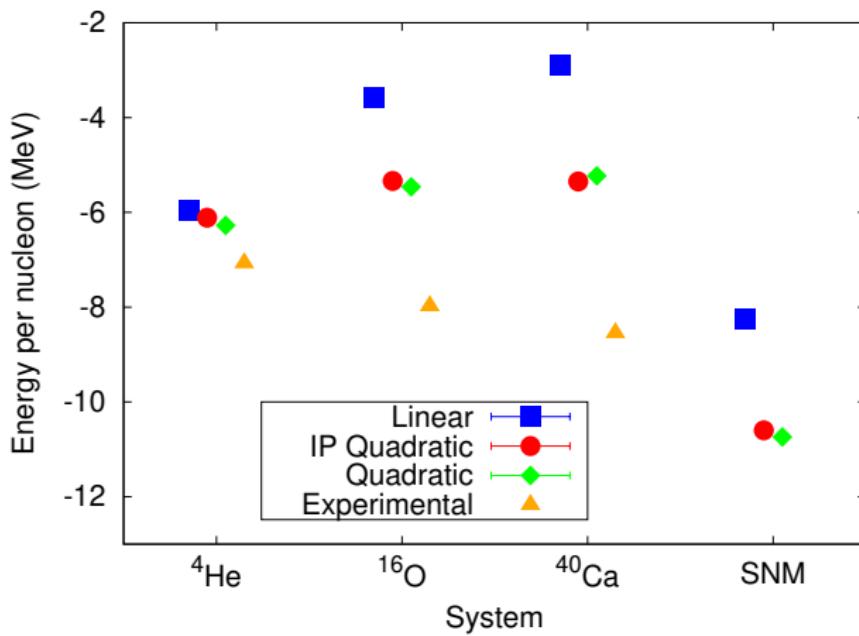


Table 1: Energy (*per nucleon) in MeV

System	Linear	IP Quadratic	Quadratic	Experimental
^4He	-27.14(4)	-27.19(3)	-27.11(3)	-28.296
^{16}O	-115.7(9)	-122.4(1.5)	-120.8(1.3)	-127.62
^{40}Ca	-322(3)	-350(10)	-351(6)	-342.1
SNM*	-13.97(3)	-14.87(4)	-14.81(3)	

Results in our recent publication (D. Lonardoni et al. *Phys. Rev. C.*, **97**, 044318, 2018).

Results - VMC

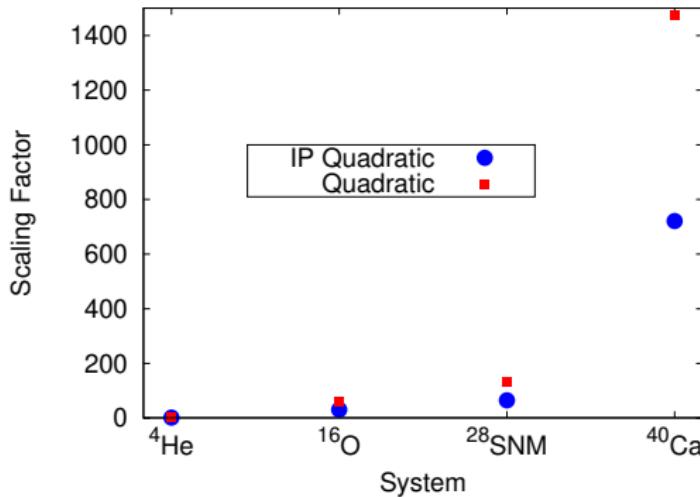


Results - χ EFT up to N²LO - Preliminary

Calculation	Correlations	⁴ He	¹⁶ O	SNM
VMC	Linear	-5.86(1)	-1.08(1)	1.56(5)
VMC	IP Quadratic	-	-4.03(4)	-
VMC	Quadratic	-6.72(1)	-3.95(4)	-
AFDMC	Linear	-6.89(2)	-5.74(4)	-9.5(1)
AFDMC	IP Quadratic	-	-7.3(2)	-12.5(1)
AFDMC	Quadratic	-6.91(2)	-6.9(2)	-12.6(1)

Note that the NN part of N²LO includes the spin-orbit interaction, which is not included in AV6' and which has been shown to decrease binding (S. Gandolfi et al. *Phys. Rev. C.*, **90**, 061306(R), 2014.).

Quadratic Correlation Cost



	^4He	^{16}O	SNM(28)	^{40}Ca
IP Quadratic	1.73	30.7	64.8	720.9
Quadratic	2.00	58.8	133.6	1473.9

Exponential Correlations

$$|\psi_T\rangle = \left[\prod_{i < j} f_c(r_{ij}) \right] e^{\sum_{i < j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p} |\phi\rangle$$

- This looks just like the propagator and so we can **use the same trick** with the HS transformation.

$$\begin{aligned} G_{SD}(R'S', RS, \Delta\tau) &= \langle R'S' | e^{-\sum_{p=2}^6 \sum_{i < j} v_p(r_{ij}) \mathcal{O}_{ij}^p \Delta\tau} | RS \rangle \\ &= \prod_{n=1}^{15A} \frac{1}{\sqrt{2\pi}} \int dx_n e^{-\frac{x_n^2}{2}} e^{\sqrt{-\lambda_n \Delta\tau} x_n O_n} \end{aligned}$$

Exponential Correlations - Preliminary

- Problems with statistical errors related to the sampling.
- Calculating the potential energy with exponential correlations and the rest with linear correlations.

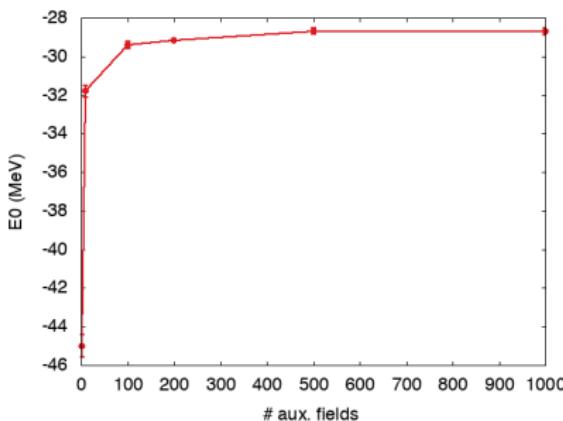


Table 2: ^4He energy with exp correlations. $E_{\text{linear}} = -26.48(9)$ MeV.

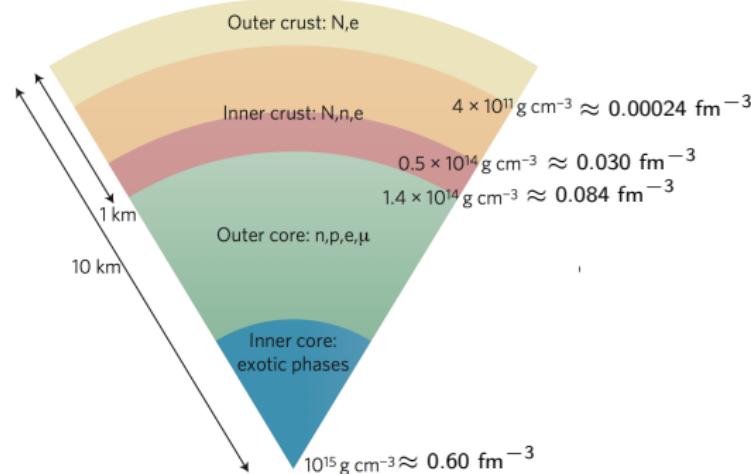
# fields	E (MeV)
1	-45.0(6)
10	-31.8(3)
100	-29.4(2)
200	-29.15(8)
500	-28.68(18)
1000	-28.7(2)

- Possible future project!

Neutron Stars - Preliminary

- Use new wave function to study α formation in the inner crust of neutron stars.

$$E_\alpha = E_{Nn+2p} - E_{(N-2)n}$$



Alpha Particle Clustering in Mostly Neutron Matter - Preliminary

- If alpha particles form in nearly neutron matter then we should be able to estimate their energy by

$$E_\alpha = E_{14n+2p} - E_{12n}$$

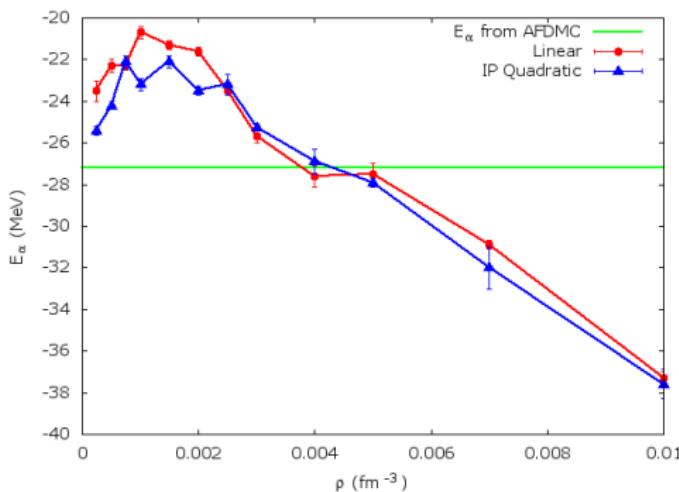
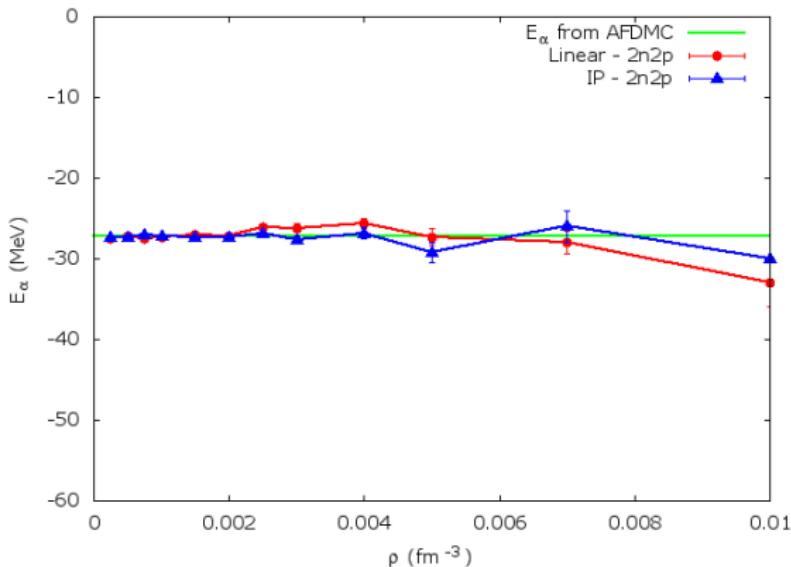


Table 3: Alpha energy in MeV - Only part of the data.

ρ (fm^{-3})	lin	ip
0.00025	-23.5(5)	-25.4(2)
0.0005	-22.3(3)	-24.2(2)
0.001	-20.7(3)	-23.2(3)
0.002	-21.6(2)	-23.5(3)
0.003	-25.7(3)	-25.26(18)
0.005	-27.5(5)	-27.9(2)
0.01	-37.3(3)	-37.6(7)

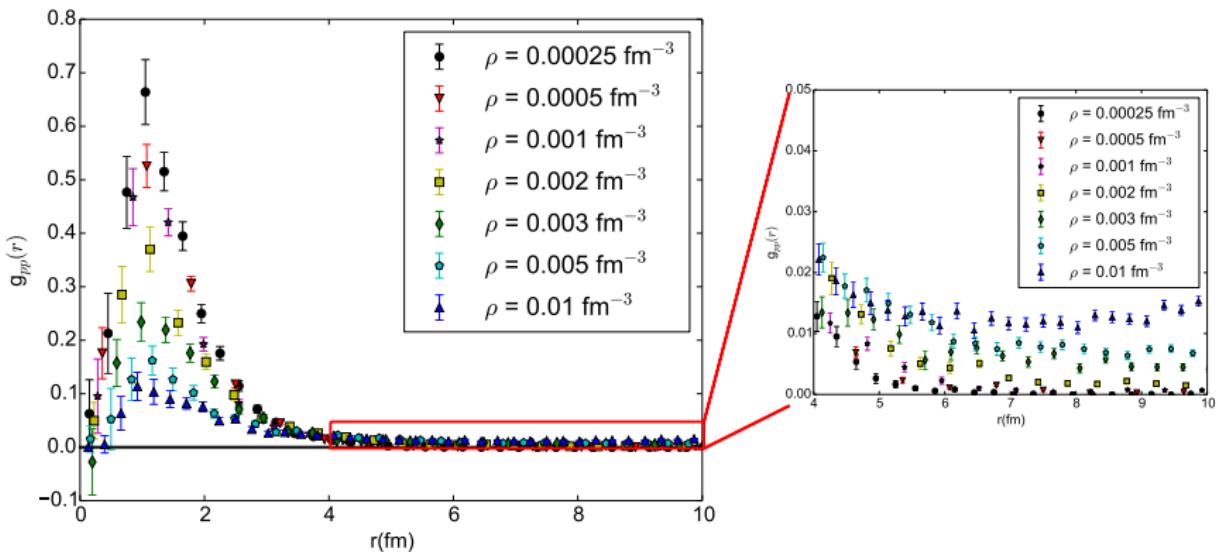
2 Protons + 2 Neutrons Only



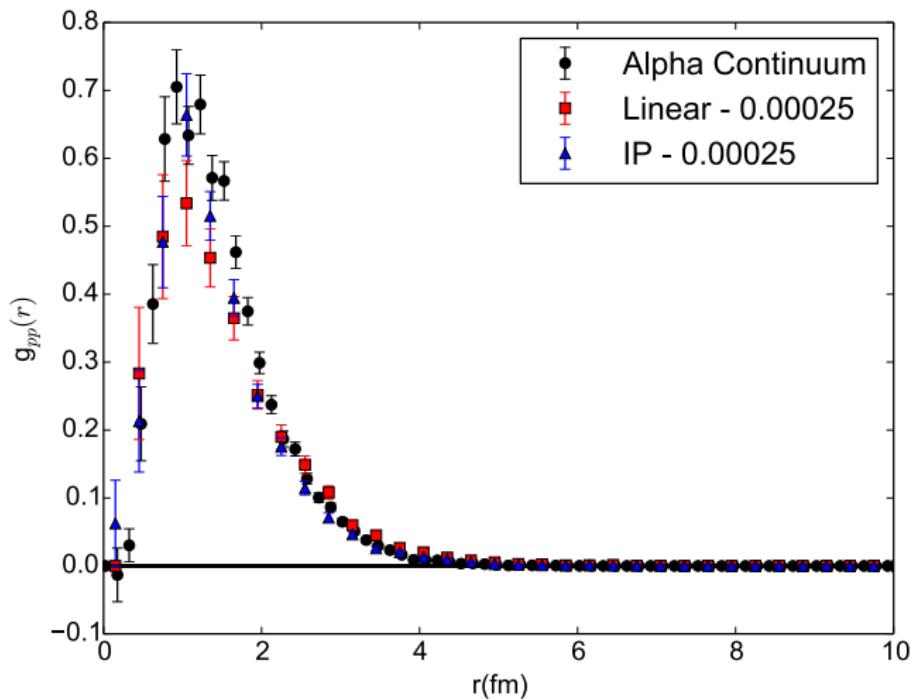
The remaining energy could be due to the α interacting with the excess neutrons.

Check for Clustering - Pair Correlation Function

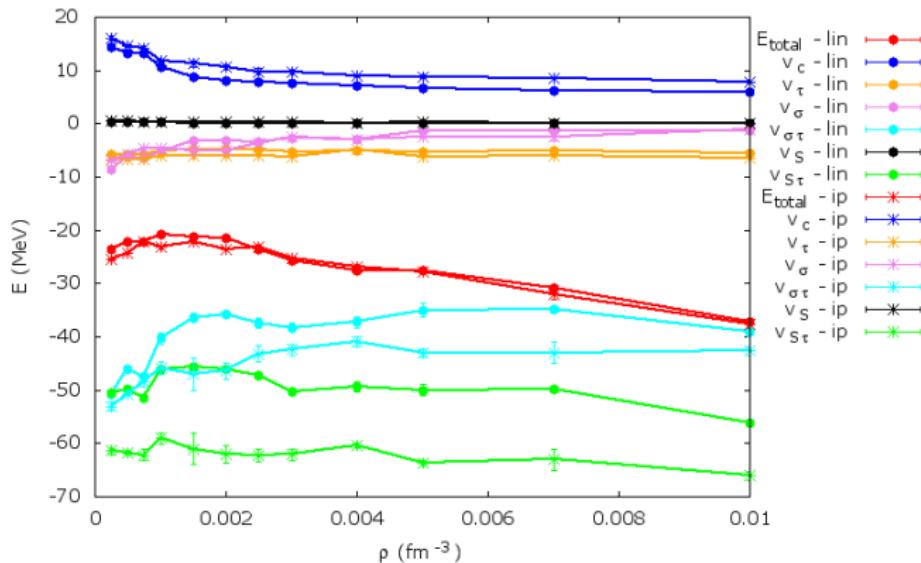
$$g_{pp}(r) = \frac{1}{4\pi r^2} \langle \Psi | \sum_{i < j} \hat{p}_i \hat{p}_j \delta(r - r_{ij}) | \Psi \rangle$$



Check for Clustering - Pair Correlation Function



Clustering - Other Insights



The tensor-tau and sigma-tau (from One Pion Exchange) are most affected by improved correlations.

Future Work

- Investigate alpha clustering with a pfaffian pairing wave function.
- Further improve the efficiency and accuracy of the trial wave function with the exponential correlations.
- Do a full investigation of both improved wave functions with the more sophisticated χ EFT potentials.

Conclusion

- AFDMC calculations need improved correlations for larger systems.
- I have improved the correlations, however, more efficient techniques are needed.
 - One possibility is to use the HS transformation with the exponential correlations.
- We can use AFDMC to study clustering in nearly neutron matter.
 - It appears that, at least at low density, the improved wave function correlations are important.

Thank You

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Extra Slides

Extra Slides

Monte Carlo Integration

- We often want to solve multidimensional integrals.

$$I = \int g(\mathbf{R}) d\mathbf{R}$$

- We can rewrite this in terms of a probability distribution $P(\mathbf{R})$.

$$I = \int f(\mathbf{R}) P(\mathbf{R}) d\mathbf{R}$$

- This looks like an expectation value of $f(\mathbf{R})$. If the \mathbf{R}_n 's are pulled from $P(\mathbf{R})$ then we can write this in discrete form as

$$I = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N f(\mathbf{R}_n) \approx \frac{1}{N} \sum_{n=1}^N f(\mathbf{R}_n)$$

Metropolis Algorithm

The Metropolis algorithm is a Markov Chain method that does not depend on history except for the previous point.

- ① Start at a random position, \mathbf{R} .
- ② Propose a move to a new position \mathbf{R}' , pulled from a distribution $T(\mathbf{R}'|\mathbf{R})$, where T could be a Gaussian centered on the current position.
- ③ One possible condition for accepting the move is given by enforcing detailed balance.

$$A(\mathbf{R}'|\mathbf{R}) = \min \left(1, \frac{P(\mathbf{R}') T(\mathbf{R}|\mathbf{R}')}{P(\mathbf{R}) T(\mathbf{R}'|\mathbf{R})} \right)$$

- ④ The move is accepted if $A \geq u$ where u is a uniform random number between 0 and 1.

χ EFT vs. AV6' with AFDMC

Table 4: Energy per nucleon in MeV calculated with AFDMC with AV6' and χ EFT up to N²LO compared to experimental data where available.

Corr	Potential	⁴ He	¹⁶ O	SNM
Linear	AV6'	-6.79(1)	-7.23(6)	-13.97(3)
	N ² LO	-6.89(2)	-5.74(4)	-9.5(1)
IP Quad	AV6'	-6.798(8)	-7.65(9)	-14.87(4)
	N ² LO	—	-7.3(2)	-12.5(1)
Quad	AV6'	-6.778(8)	-7.55(8)	-14.81(3)
	N ² LO	-6.91(2)	-6.9(2)	-12.6(1)
Experimental		-7.074	-7.98	

χ EFT vs. AV6' with VMC

Table 5: Energy per nucleon in MeV calculated with VMC with AV6' and χ EFT up to N²LO.

Corr	Potential	⁴ He	¹⁶ O	SNM
Linear	AV6'	-5.96(1)	-3.581(3)	-8.25(4)
	N ² LO	-5.86(1)	-1.08(1)	1.56(5)
IP Quad	AV6'	-6.113(8)	-5.338(3)	-10.60(3)
	N ² LO	—	-4.03(4)	—
Quad	AV6'	-6.275(5)	-5.463(3)	-10.74(2)
	N ² LO	-6.72(1)	-3.95(4)	—

Exponential Correlations - Problems

- When taking numerical derivatives the order of A matrix eigenvectors (given by n) can change. This means that each term in the derivative can have each eigenvector matched with a different auxiliary field.

$$\exp \left(\sum_{i < j, p} f_p(r_{ij}) \mathcal{O}_{ij}^p \right) = \prod_{n=1}^{15A} \frac{1}{\sqrt{2\pi}} \int dx_n e^{-x_n^2/2} e^{\sqrt{\lambda_n} x_n O_n}$$

- To fix this we can define the operators O_n in terms of the square roots of the A matrices. This gives an operator that sums over the eigenvector order.

Exponential Correlations - Problems

- Just Almost like before

$$\begin{aligned} \exp \left(\sum_{i < j, p} f_p(r_{ij}) \mathcal{O}_{ij}^p \right) = & \exp \left(\frac{1}{2} \sum_{i\alpha, j\beta} \sigma_{i\alpha} \sum_{k\gamma} (A_{i\alpha, k\gamma}^\sigma)^{1/2} (A_{k\gamma, j\beta}^\sigma)^{1/2} \sigma_{j\beta} \right. \\ & + \frac{1}{2} \sum_{i\alpha, j\beta} \sigma_{i\alpha} \sum_{k\gamma} (A_{i\alpha, k\gamma}^{\sigma\tau})^{1/2} (A_{k\gamma, j\beta}^{\sigma\tau})^{1/2} \sigma_{j\beta} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \\ & \left. + \frac{1}{2} \sum_{i,j} \sum_k (A_{i,k}^\tau)^{1/2} (A_{k,j}^\tau)^{1/2} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \right) \end{aligned}$$

Exponential Correlations - Problems

$$\exp \left(\sum_{i < j, p} f_p(r_{ij}) \mathcal{O}_{ij}^p \right) = \exp \left(\frac{1}{2} \sum_{k\delta=1}^{3A} (O_{k\delta}^\sigma)^2 + \frac{1}{2} \sum_{\gamma=1}^3 \sum_{k\delta=1}^{3A} (O_{k\delta,\gamma}^{\sigma\tau})^2 + \frac{1}{2} \sum_{\gamma=1}^3 \sum_{k=1}^A (O_{k,\gamma}^\tau)^2 \right)$$

$$O_{k\delta}^\sigma = \sum_{i\alpha} \sum_n \sigma_{i\alpha} \psi_{n,i\alpha}^\sigma (\lambda_n^\sigma)^{1/2} \psi_{n,k\delta}^\sigma$$

$$O_{k\delta,\gamma}^{\sigma\tau} = \sum_{i\alpha} \sum_n \tau_{i\gamma} \sigma_{i\alpha} \psi_{n,i\alpha}^{\sigma\tau} (\lambda_n^{\sigma\tau})^{1/2} \psi_{n,k\delta}^{\sigma\tau}$$

$$O_{k\delta}^\tau = \sum_i \sum_n \tau_{i\gamma} \psi_{n,i}^\tau (\lambda_n^\tau)^{1/2} \psi_{n,k}^\tau$$

Two-Body Operator Updates

$$S = \begin{pmatrix} \langle \alpha_1 | \mathbf{r}_1, s_1 \rangle & \langle \alpha_1 | \mathbf{r}_2, s_2 \rangle & \dots & \langle \alpha_1 | \mathbf{r}_A, s_A \rangle \\ \langle \alpha_2 | \mathbf{r}_1, s_1 \rangle & \langle \alpha_2 | \mathbf{r}_2, s_2 \rangle & \dots & \langle \alpha_2 | \mathbf{r}_A, s_A \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \alpha_A | \mathbf{r}_1, s_1 \rangle & \langle \alpha_A | \mathbf{r}_2, s_2 \rangle & \dots & \langle \alpha_A | \mathbf{r}_A, s_A \rangle \end{pmatrix}$$

$$S_{\alpha i} = \langle \alpha | \mathbf{r}_i, s_i \rangle = \sum_{\gamma=1}^4 \langle \alpha | \mathbf{r}_i \chi_\gamma \rangle \langle \chi_\gamma | s_i \rangle .$$

This is for an uncorrelated Slater Determinant.

Two-Body Operator Updates

When correlation operators are included we employ the identity

$$\det(S^{-1}S') = \frac{\det S'}{\det S} \quad \text{or} \quad \det(S^{-1}S'') = \frac{\det S''}{\det S}$$

where

$$S^{-1}S'' = \begin{pmatrix} 1 & 0 & \dots & \langle \alpha_1 | \mathcal{O}_i | \mathbf{r}_i, s_i \rangle & \dots & \langle \alpha_1 | \mathcal{O}_j | \mathbf{r}_j, s_j \rangle & \dots & 0 & 0 \\ 0 & 1 & \dots & \langle \alpha_2 | \mathcal{O}_i | \mathbf{r}_i, s_i \rangle & \dots & \langle \alpha_2 | \mathcal{O}_j | \mathbf{r}_j, s_j \rangle & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & \langle \alpha_A | \mathcal{O}_i | \mathbf{r}_i, s_i \rangle & \dots & \langle \alpha_A | \mathcal{O}_j | \mathbf{r}_j, s_j \rangle & \dots & 0 & 1 \end{pmatrix}$$

and

$$\det S^{-1}S'' = \det \begin{pmatrix} \langle \alpha_i | \mathcal{O}_i | \mathbf{r}_i, s_i \rangle & \langle \alpha_i | \mathcal{O}_j | \mathbf{r}_j, s_j \rangle \\ \langle \alpha_j | \mathcal{O}_i | \mathbf{r}_i, s_i \rangle & \langle \alpha_j | \mathcal{O}_j | \mathbf{r}_j, s_j \rangle \end{pmatrix}$$

Two-Body Operator Updates

In practice this is done by calculating

$$\frac{\langle \Phi | \mathcal{O}_{ij} | RS \rangle}{\langle \Phi | RS \rangle} = \sum_{\gamma=1}^4 \sum_{\delta=1}^4 d_{2b}(\chi_\gamma, \chi_\delta, ij) \langle \chi_\gamma \chi_\delta | \mathcal{O}_{ij} | s_i s_j \rangle,$$

where

$$d_{2b}(\chi_\gamma, \chi_\delta, ij) = \frac{\langle \Phi | R, s_1, \dots, s_{i-1}, \chi_\gamma, s_{i+1}, \dots, s_{j-1}, \chi_\delta, s_{j+1}, \dots, s_A \rangle}{\langle \Phi | RS \rangle}.$$

Two-Body Operator Updates

To reduce the number of calculations in the inner loops we precalculate the matrix elements

$$P_{\chi_\gamma,ij} = \sum_\alpha S_{j\alpha}^{-1} S_{\alpha i}(s_i \leftarrow \chi_\gamma),$$

$$P_{\chi_\delta,ij} = \sum_\alpha S'_{j\alpha}^{-1} S'_{\alpha i}(s_j \leftarrow \chi_\delta).$$

The d_{2b} distribution can then be written as

$$d_{2b}(\chi_\gamma, \chi_\delta, ij) = \det \begin{pmatrix} P_{\chi_\gamma,ii} & P_{\chi_\gamma,ij} \\ P_{\chi_\delta,ji} & P_{\chi_\delta,jj} \end{pmatrix}$$

The d_{2b} can be precalculated and multiplied by each operator expectation value $\langle \chi_\gamma \chi_\delta | \mathcal{O}_{ij} | s_i s_j \rangle$.

Two-Body Operator Updates - Scaling

Calculation	Functional Form	Scaling
Ψ (linear)	$\mathbb{1} + \mathcal{O}_{ij}^c$	$O(A^2)$
Ψ (quadratic)	$\mathbb{1} + \mathcal{O}_{ij}^c + \mathcal{O}_{ij}^c \mathcal{O}_{kl}^c$	$O(A^4)$
$\langle H \rangle$ (linear)	$\left(\mathbb{1} + \mathcal{O}_{ij}^c \right) \mathcal{O}_{mn}^p$	$O(A^4)$
$\langle H \rangle$ (quadratic)	$\left(\mathbb{1} + \mathcal{O}_{ij}^c + \mathcal{O}_{ij}^c \mathcal{O}_{kl}^c \right) \mathcal{O}_{mn}^p$	$O(A^6)$

Forward Walking

- Mixed estimators contain bias from Ψ_T

$$\langle \mathcal{O} \rangle_p \approx 2 \langle \mathcal{O} \rangle_{mixed} - \langle \mathcal{O} \rangle_{VMC}$$

$$\langle \mathcal{O} \rangle_{mixed} = \frac{\langle \Psi_T | \mathcal{O} | \Psi(\tau) \rangle}{\langle \Psi_T | \Psi(\tau) \rangle}$$

- Some of this can be removed with a “forward walking” scheme

$$\begin{aligned}\langle \mathcal{O} \rangle_p &= \frac{\langle \Psi(\tau) | \mathcal{O} | \Psi(\tau) \rangle}{\langle \Psi(\tau) | \Psi(\tau) \rangle} = \frac{\langle \Psi_T | \frac{\Psi(\tau)}{\Psi_T} \mathcal{O} | \Psi(\tau) \rangle}{\langle \Psi_T | \frac{\Psi(\tau)}{\Psi_T} | \Psi(\tau) \rangle} \\ &= \frac{\sum_i \mathcal{O}_i W_i}{\sum_i W_i}\end{aligned}$$

i are the random samples (walkers).

VMC - Parameter Variation

- The updated wave function can be written, up to linear order, as

$$|\psi_T(\alpha + \Delta\alpha)\rangle = |\psi_T(\alpha)\rangle + \sum_{k=1}^p \Delta\alpha_k \frac{\partial}{\partial\alpha_k} |\psi_T(\alpha)\rangle + \dots$$

- Or in a more compact way as

$$|\psi_T(\alpha + \Delta\alpha)\rangle = \sum_{k=0}^p \Delta\alpha_k \mathcal{O}_k |\psi_T(\alpha)\rangle,$$

where

$$\mathcal{O}_k = \frac{\partial \ln \psi_\alpha}{\partial \alpha_k} = \frac{\partial_{\alpha_k} \psi_\alpha}{\psi_\alpha}$$

- Then just find the optimal values of $\Delta\alpha_k$.

VMC - Parameter Variation - Stochastic Reconfiguration

- This is done similar to Lanczos method

$$|\psi'_T\rangle = (\Lambda \mathbb{1} - H) |\psi_T\rangle,$$

- Using these you can write down the SR condition

$$\langle\psi_T| \mathcal{O}_k(\Lambda \mathbb{1} - H) |\psi_T\rangle = \langle\psi_T| \mathcal{O}_k |\psi'_T\rangle$$

- Which can be written as a linear system and the $\Delta\alpha_k$ solved for

$$\sum_i \Delta\alpha_i s_{i,k} = f^k$$

where

$$s_{i,k} = \sum_x \langle\psi_T| \mathcal{O}_x^i \mathcal{O}_x^k |\psi_T\rangle$$

$$f^k = \langle\psi_T| \mathcal{O}_k(\Lambda \mathbb{1} - H) |\psi_T\rangle$$

Pfaffian Wave Function

$$\Psi_{BCS}(\mathbf{RS}) = \mathcal{A} [\phi(\mathbf{r}_1, s_1, \mathbf{r}_2, s_2) \phi(\mathbf{r}_3, s_3, \mathbf{r}_4, s_4) \dots \phi(\mathbf{r}_{A-1}, s_{A-1}, \mathbf{r}_A, s_A)]$$

- The spin parts can be written in terms of singlet and triplet states.
- Developed to describe low energy Cooper pairs and superconductivity.
- Can be calculated in $\mathcal{O}(A^3)$ operations just like a determinant.

Tensor Force

$$S_{ij} = 3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$$

- The tensor force describes the relationship of two spins given their relative position

