

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

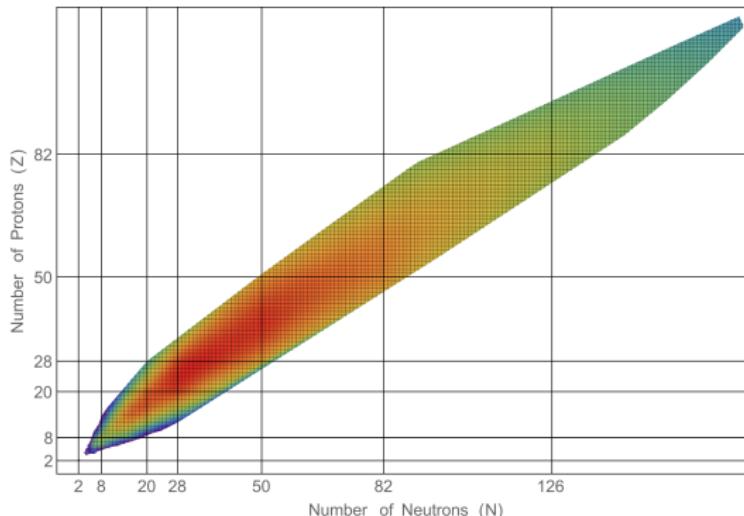
## 3 Conclusion

- 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.
- The variational principle guarantees

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

- We want this to look like this

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

# Variational Monte Carlo

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

- We can do that if we multiply by  $\Psi_T(\mathbf{R})\Psi_T^{-1}(\mathbf{R})$ .

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

- 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.

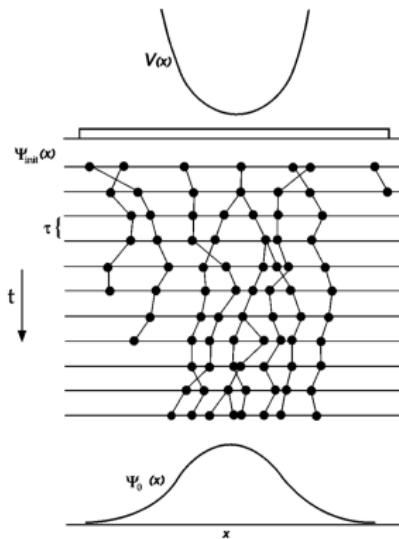
$$w(\mathbf{R}') = e^{-(V(\mathbf{R}') + V(\mathbf{R}) - 2E_0)\Delta\tau/2}$$

- 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  $\xi$  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.

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

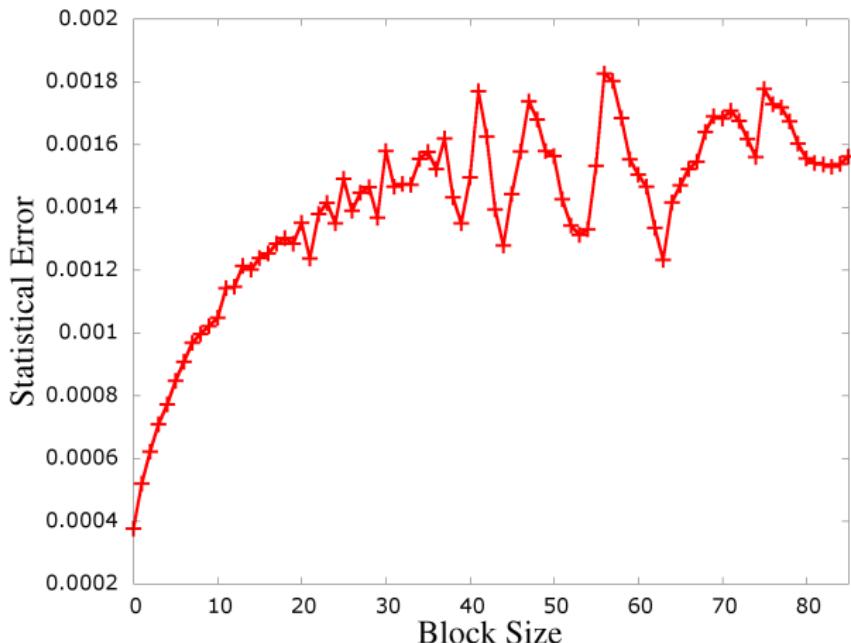
$$\langle \mathcal{O} \rangle_{\text{mixed}} = \frac{\langle \Psi(\tau) | \mathcal{O} | \Psi_T \rangle}{\langle \Psi(\tau) | \Psi_T \rangle}, \quad \langle \mathcal{O} \rangle_{\text{VMC}} = \frac{\langle \Psi_T | \mathcal{O} | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$$

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

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

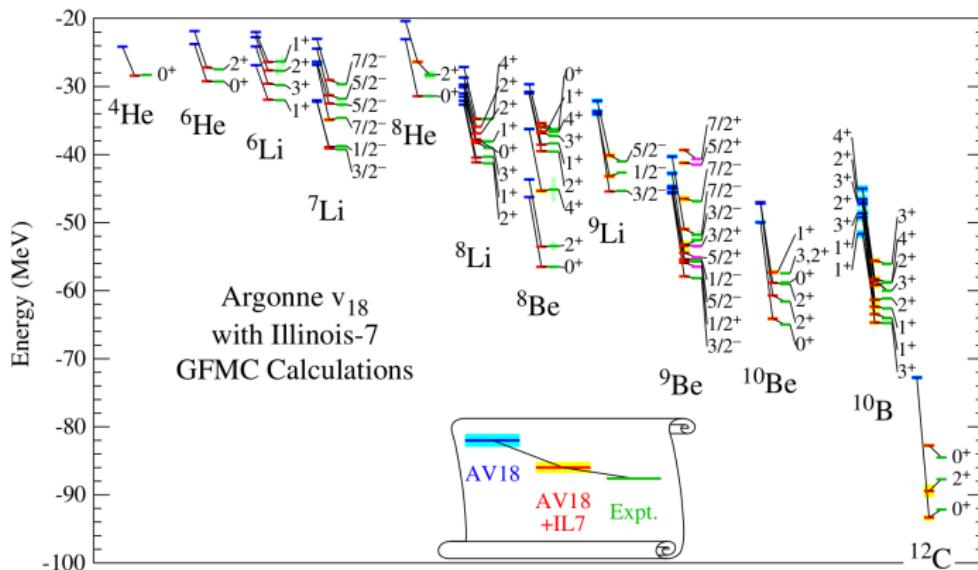
# Estimating Error

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

- 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

- To avoid explicitly doing the  $2^A \frac{A!}{Z!(A-Z)!}$  sums over the spin-isospin states AFDMC writes the spin-isospin dependent propagator in terms of squared single particle operators.
- The spin-isospin dependent operators

$$e^{-V_{SD}\Delta\tau}$$

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

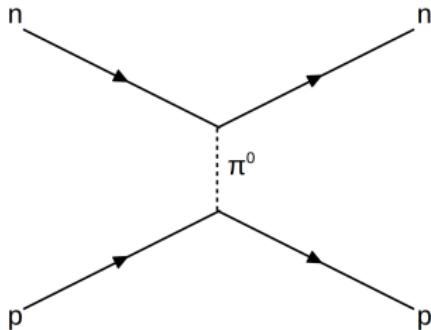
- We have squared single particle operators in the propagator we can now rewrite the propagator in terms of the Hubbard-Stratanovich transformation.

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

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

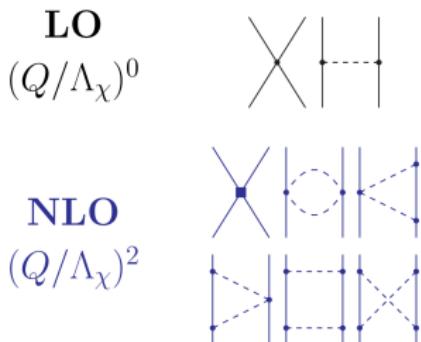
$$G_{SD}(R'S', RS, \Delta\tau) = \prod_{n=1}^{15A} \frac{1}{\sqrt{2\pi}} \int dx_n e^{-\frac{x_n^2}{2}} e^{\sqrt{-\lambda_n \Delta\tau} x_n O_n}.$$

# Hamiltonian



Based on meson exchange

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



Based on  $\chi$ EFT expansion in momentum (up to  $N^2LO$ )

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  $\chi$ EFT NN and 3N potentials up to N<sup>2</sup>LO.
- First 6 operators of the AV18 potential

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

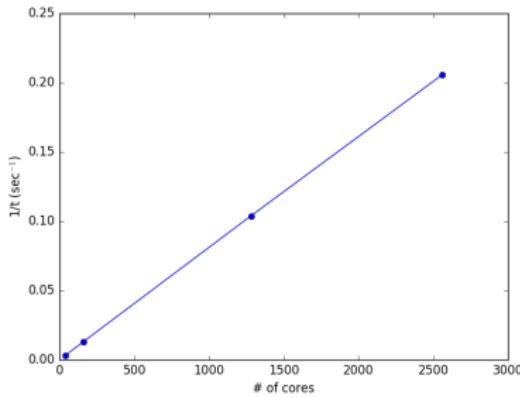
$$\mathcal{O}_{ij}^p = 1, \ \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j, \ \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, \ \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j, \ S_{ij}, \ S_{ij} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$$

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

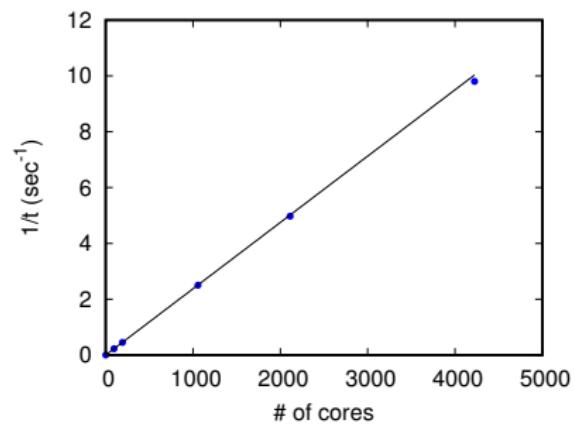
# Scaling

- 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  $^{16}\text{O}$  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.



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

- 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.

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

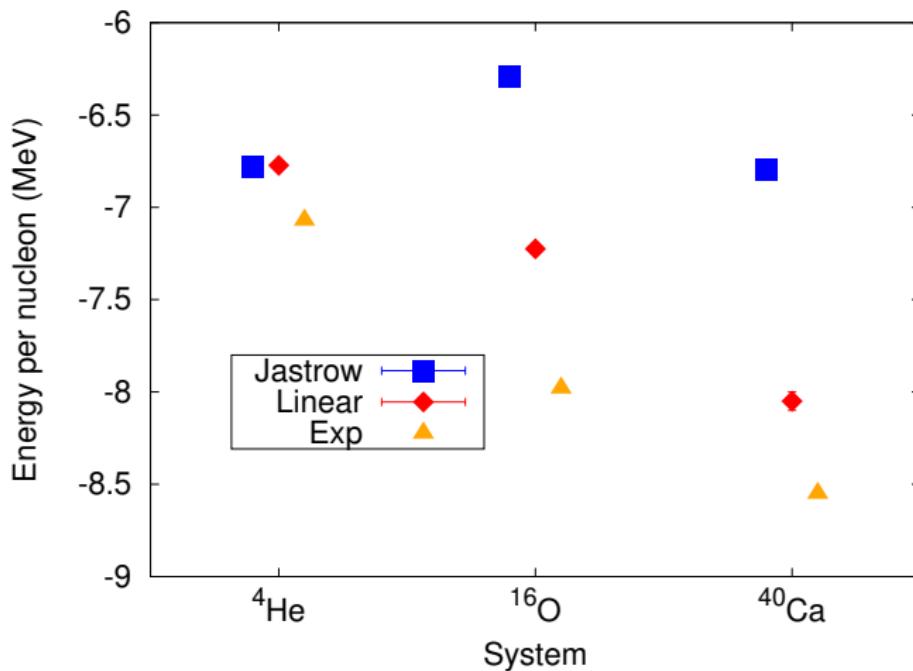
S. Gandolfi et al. *Phys. Rev. Lett.*, **99**, 022507, 2007.

- 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

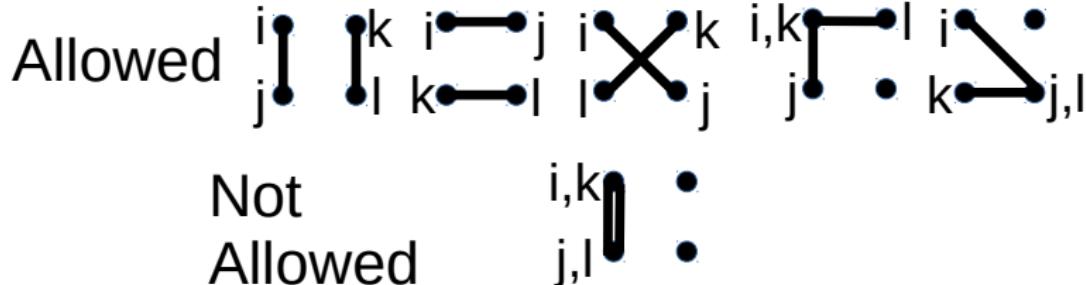


Data taken from each paper respectively.

# Symmetrized Product Wave Function

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

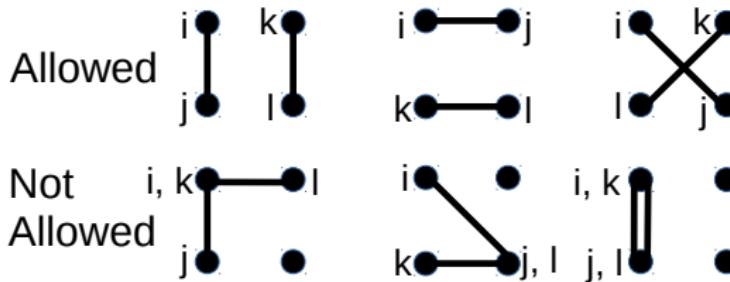
$$|\psi_T\rangle = \left[ \prod_{i < j} f_c(r_{ij}) \right] \left[ 1 + \sum_{i < j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p + \frac{1}{2} \sum_{i < j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p \sum_{\substack{k < l \\ ij \neq kl}} \sum_q f_q(r_{kl}) \mathcal{O}_{kl}^q \right] |\phi\rangle$$



# Independent Pair Quadratic Correlations

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

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



## Results - AFDMC

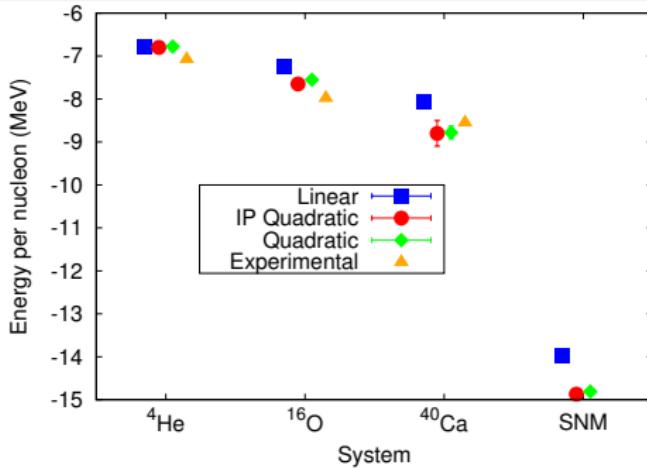
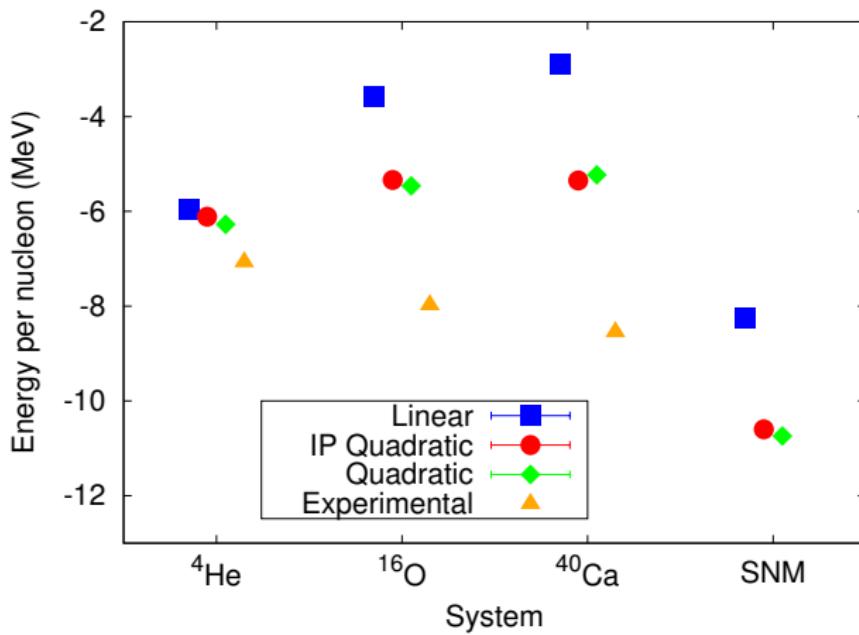


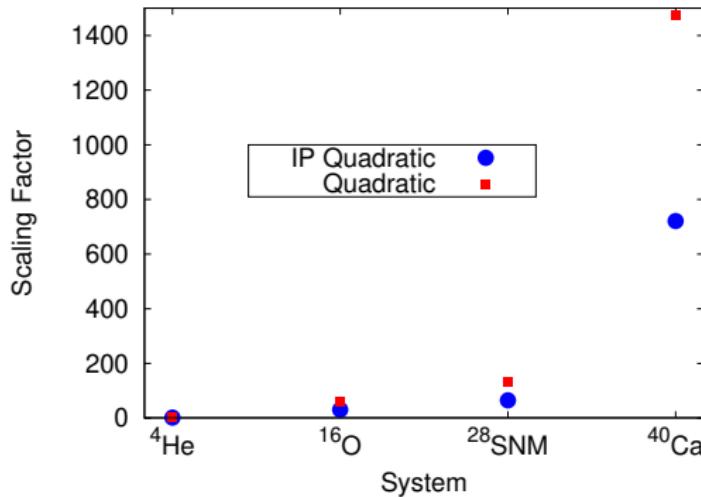
Table 1 : Energy (\*per nucleon) in MeV

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

## Results - VMC



# Quadratic Correlation Cost



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

Results -  $\chi$ EFT up to N<sup>2</sup>LO - Preliminary

Calculation	Correlations	$^4\text{He}$	$^{16}\text{O}$	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 N<sup>2</sup>LO 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.).

# 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.

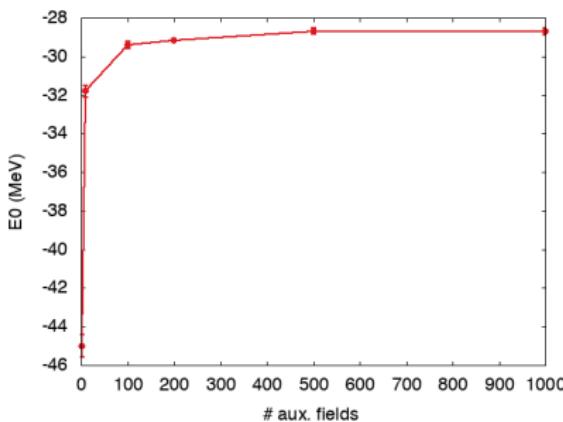


Table 2 :  $^4\text{He}$  energy with exp correlations.  $E_{\text{linear}} = -26.48(9)$  MeV.

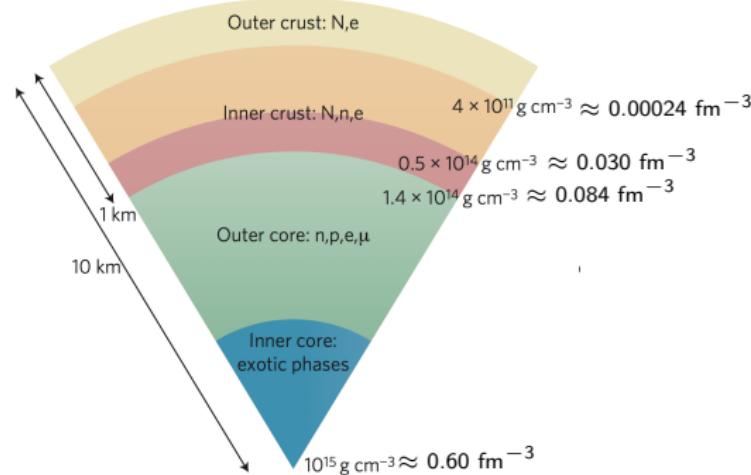
# fields	E (MeV)
1	-45.0(6)
10	-31.8(3)
100	-29.4(2)
200	-29.15(8)
500	-28.68(18)
1000	-28.7(2)

- Possible future project!

# Neutron Stars - Preliminary

- Use new wave function to study  $\alpha$  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

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

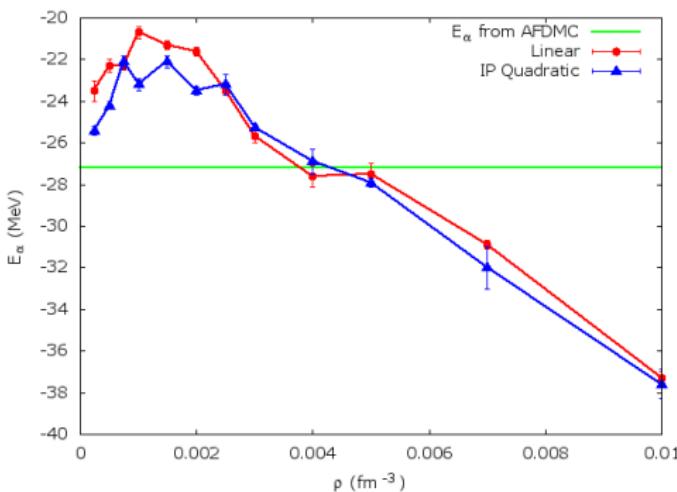
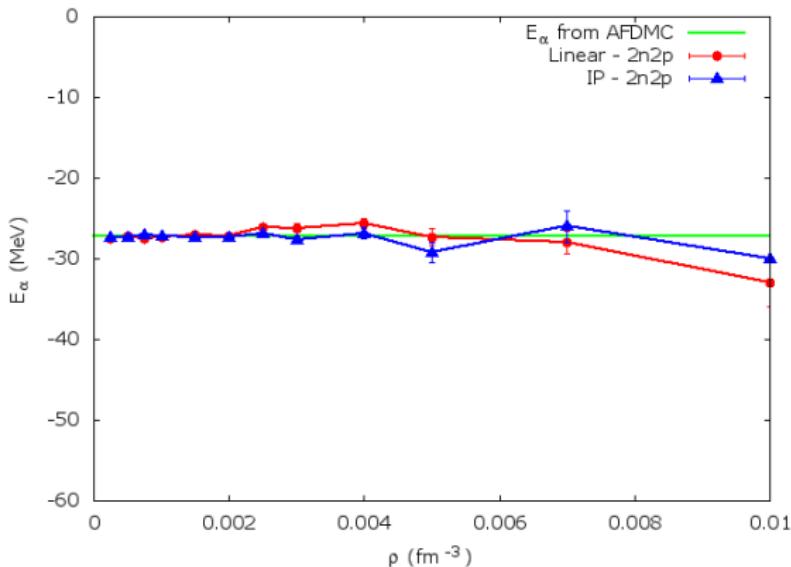


Table 3 : Alpha energy in MeV - Only part of the data.

$\rho$ (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)

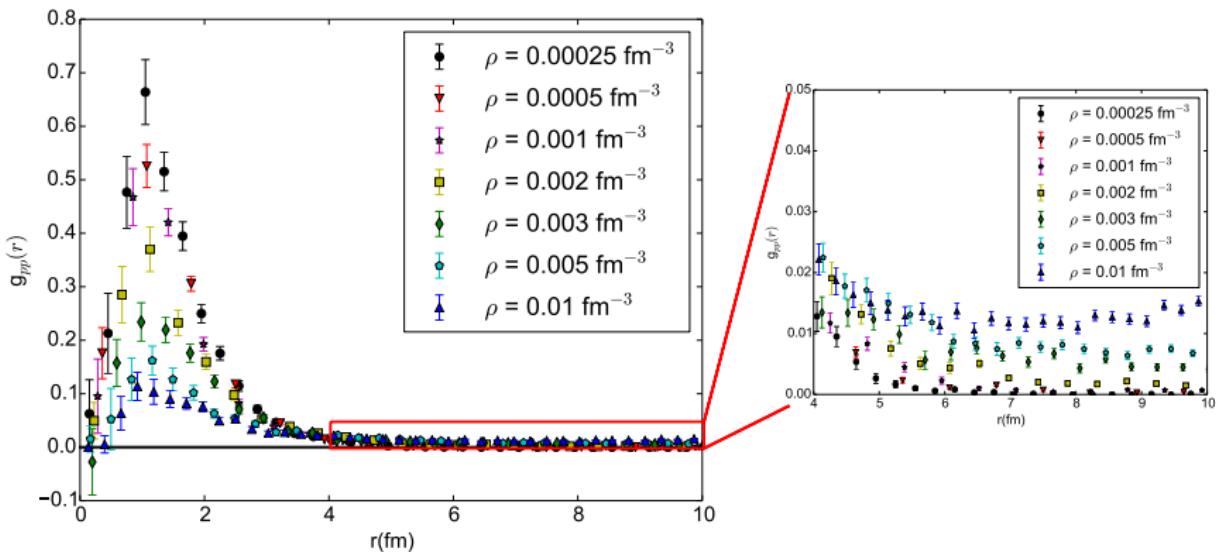
## 2 Protons + 2 Neutrons Only



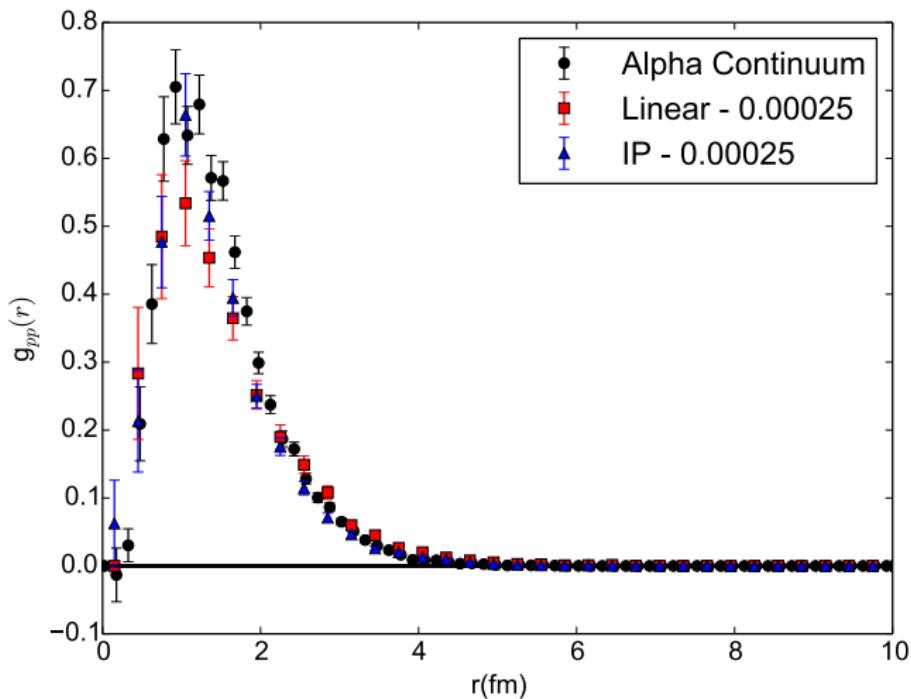
The remaining energy could be due to the  $\alpha$  interacting with the excess neutrons.

## Check for Clustering - Pair Correlation Function

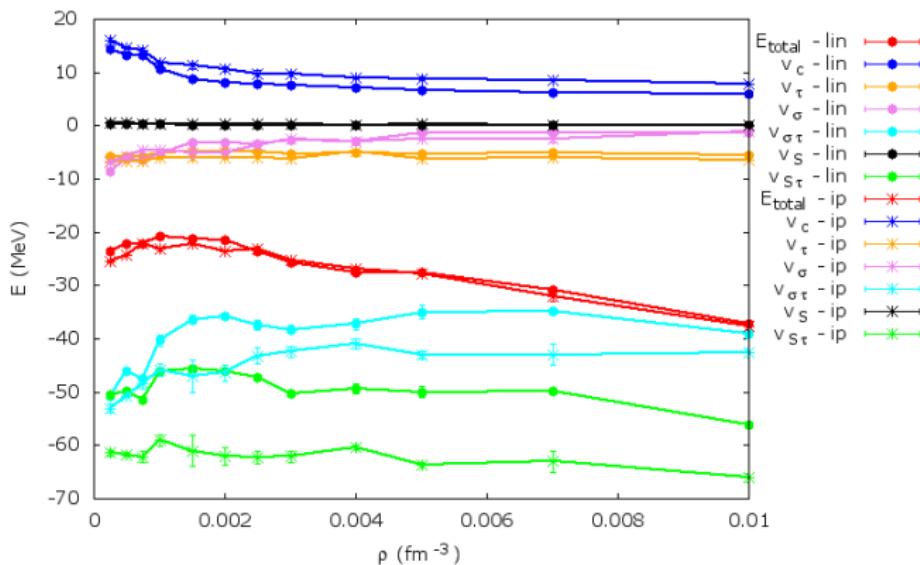
$$g_{pp}(r) = \frac{1}{4\pi r^2} \langle \Psi | \sum_{i < j} \hat{p}_i \hat{p}_j \delta(r - r_{ij}) | \Psi \rangle$$



## Check for Clustering - Pair Correlation Function



## Clustering - Other Insights



The tensor-tau and sigma-tau (from OPE) 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  $\chi$ EFT potentials.

# Conclusion

- AFDMC calculations need to 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 a low density, the improved wave function correlations are important.

# Thanks

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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.

# $\chi$ EFT vs. AV6' with AFDMC

Table 4 : Energy per nucleon in MeV calculated with AFDMC with AV6' and  $\chi$ EFT up to N<sup>2</sup>LO compared to experimental data where available.

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

# $\chi$ EFT vs. AV6' with VMC

**Table 5 :** Energy per nucleon in MeV calculated with VMC with AV6' and  $\chi$ EFT up to N<sup>2</sup>LO.

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

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

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

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

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

# VMC - Parameter Variation

EXPLAIN HOW THE PARAMETARS ARE VARIED IN VMC.

# Pfaffian Wave Function

FINISH THIS! Maybe call it the BCS wave function, which we calculate as a pfaffian of paired orbitals.

# Alpha Clusters

WHY ARE CLUSTERS IMPORTANT? ARE THEY NORMALLY DONE WITH SOME MODEL, NOT AB INITIO LIKE WE ARE DOING? ARE THEY AT LEAST WRITTEN IN TERMS OF P, N, AND ALPHA DEGREES OF FREEDOM? WE ARE ONLY USING N AND P.