

# 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

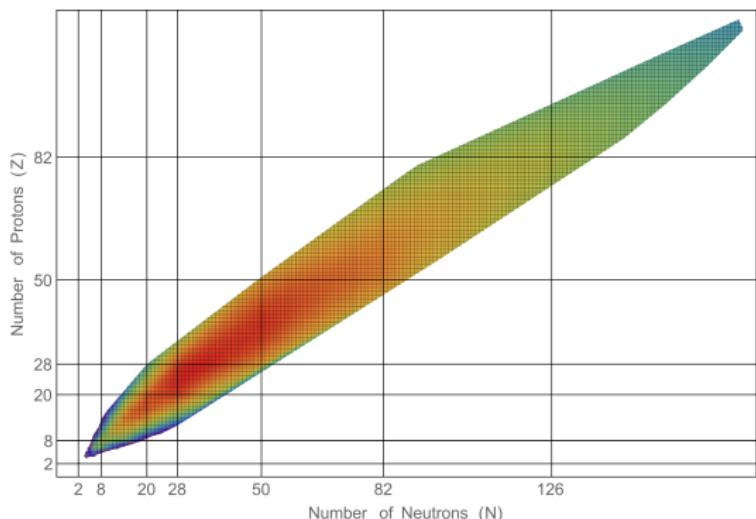
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## └ Outline

# Nuclear Many Body Problem

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

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



## Motivation

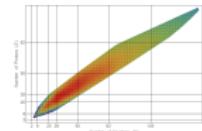
### Nuclear Many Body Problem

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- Many-body quantum problem with  $n$  and  $p$  dof.
- GROUND STATE properties.
- Up to  $^{40}\text{Ca}$  and  $\sim A=100$  for nuclear matter.
- Show on the chart up to where our method is applicable.
- Integrals infeasible to do using standard stuff, so we use MC.

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# 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

## Motivation

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# Variational Monte Carlo

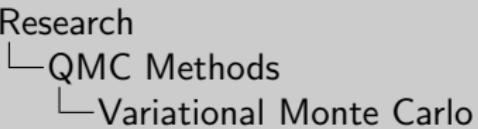
- VMC starts with a trial wave function which includes variable parameters.
- Variational energy is an upper bound to the ground state energy.

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

- Integral is solved with MC integration.

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

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# Variational Monte Carlo

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

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

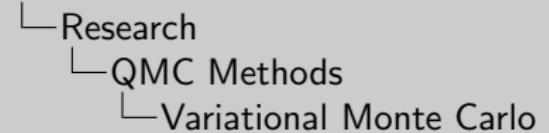
$$P(\mathbf{R}) = \frac{|\Psi_T(\mathbf{R})|^2}{\int |\Psi_T(\mathbf{R})|^2 d\mathbf{R}}, \quad E_L(\mathbf{R}) = \frac{\Psi_T^*(\mathbf{R}) H \Psi_T(\mathbf{R})}{\Psi_T^*(\mathbf{R}) \Psi_T(\mathbf{R})}$$

- 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  $P(\mathbf{R})$ .

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## 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  $E_V \geq E_0$ .

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# 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.

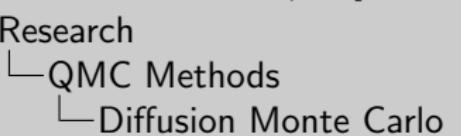
$$H\Psi = i\hbar \frac{d\Psi}{dt} \xrightarrow{\tau=it/\hbar} H\Psi = -\frac{d\Psi}{d\tau}$$

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.

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



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- We start DMC from the minimized  $\psi_T$  and configurations from VMC.
- Description is only for SPATIAL coordinates, not SPINS yet.

## Diffusion Monte Carlo

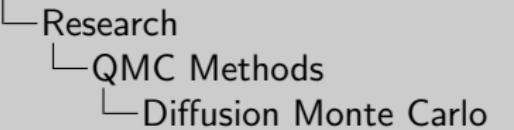
- The propagated wave function can be written

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

- 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  $\Delta\tau = \tau/N$ .

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

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- In practice: Green's function (propagator).
- Can't do full time propagation.
- Can do short time propagation.
- Stress the importance of having an accurate and "cheap" wave function.

# 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.

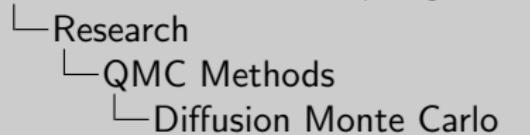
$$\langle \mathbf{R}' | e^{-T\Delta\tau} | \mathbf{R} \rangle = \left( \frac{m}{2\pi\hbar^2\Delta\tau} \right)^{3A/2} e^{-m(\mathbf{R}'-\mathbf{R})^2/2\hbar^2\Delta\tau}$$

- 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

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



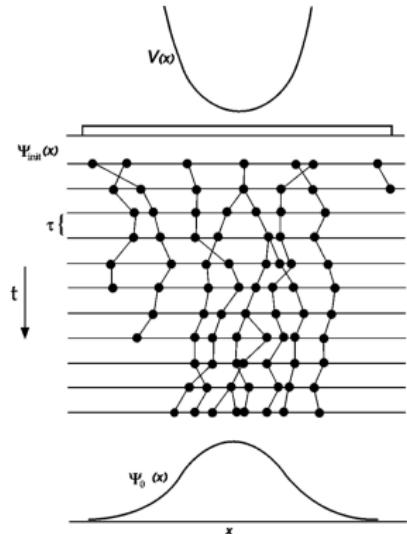
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# Diffusion Monte Carlo - Branching

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.

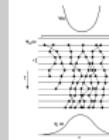


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- Branching eliminates repeated cycles.
- To avoid carrying insignificant walkers through the calculation.

# 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  $[\mathcal{O}, H]=0$

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

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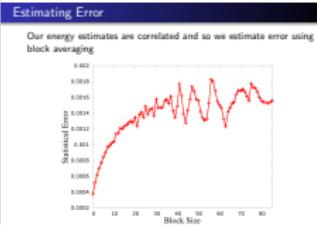
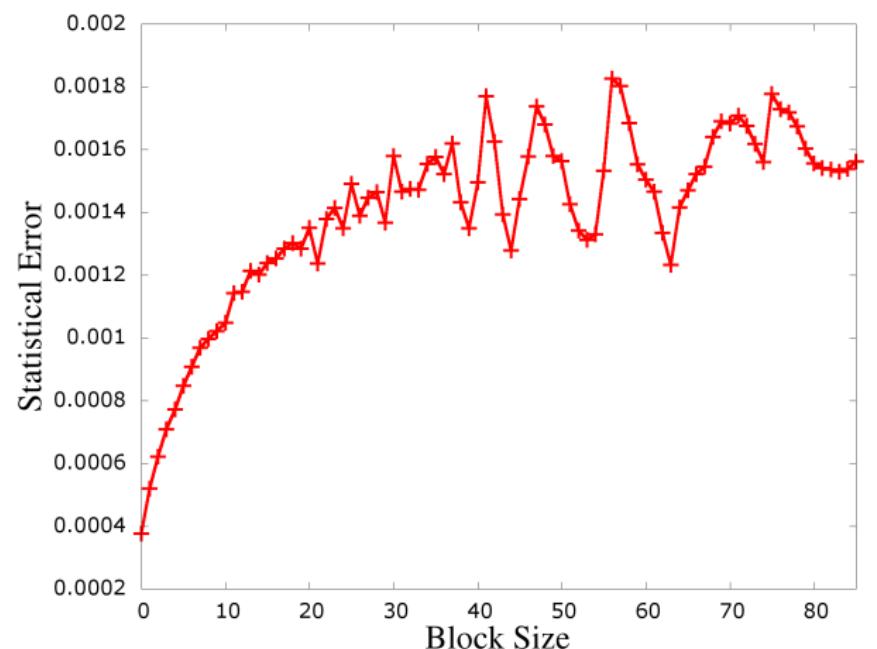
In the large  $\tau$  limit when  $[\mathcal{O}, H]=0$

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- It's difficult to operate through the propagator.
- Accurate to  $\mathcal{O}[(\psi(\tau) - \psi_T)^2]$
- This could be done with **forward walking** but it typically isn't necessary.

# Estimating Error

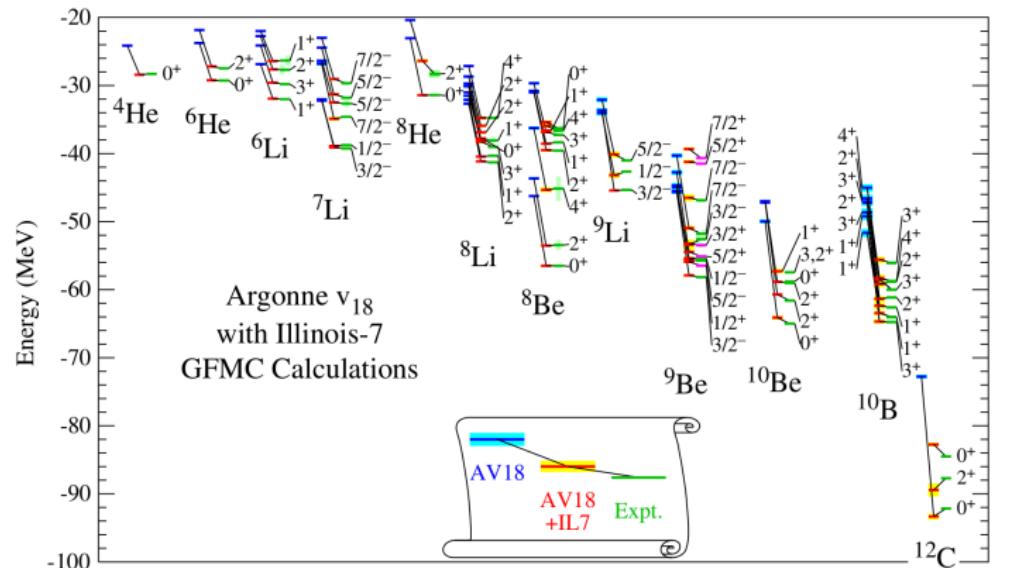
Our energy estimates are correlated and so we estimate error using block averaging



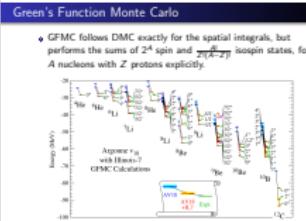
- We don't usually (though you could) talk about the uncertainty in the statistical errors. It's the wiggles at the plateau. We just report 1 digit.

# 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.



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- The excited states come by changing the  $J^\pi$  and  $T$  of the wave function.

# 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  $S_{ij} = 3\sigma_i \cdot \hat{r}_{ij} \sigma_j \cdot \hat{r}_{ij} - \sigma_i \cdot \sigma_j$

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# Auxiliary Field Diffusion Monte Carlo - Spin Sampling

- The spin-isospin dependent operators

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is sampled by using the Hubbard-Stratanovich transformation.

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

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# 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.

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

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

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# Auxiliary Field Diffusion Monte Carlo - Spin Sampling

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

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

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

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# 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

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

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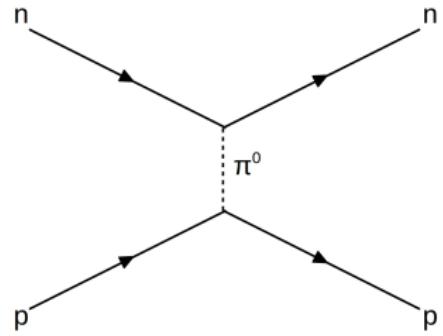
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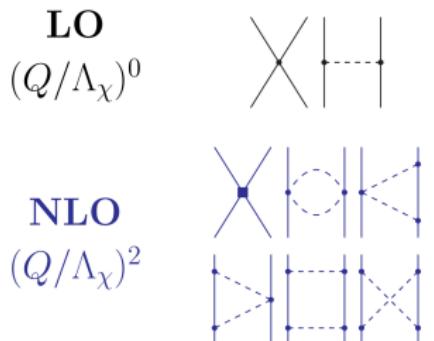
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# Hamiltonian



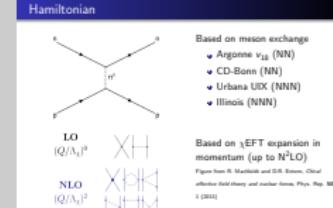
Based on meson exchange

- 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

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

$$\mathcal{O}_{ij}^p = 1, \tau_i \cdot \tau_j, \sigma_i \cdot \sigma_j, \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j, S_{ij}, S_{ij} \tau_i \cdot \tau_j$$

$$S_{ij} = 3\sigma_i \cdot \hat{r}_{ij} \sigma_j \cdot \hat{r}_{ij} - \sigma_i \cdot \sigma_j$$

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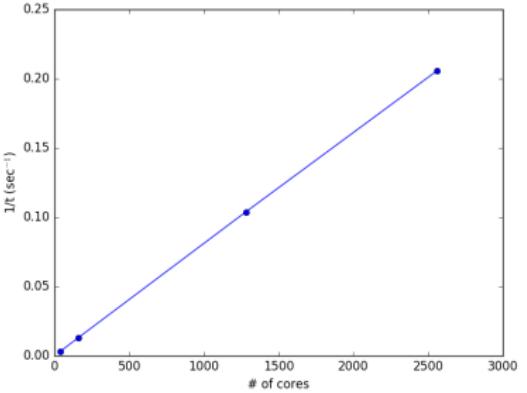
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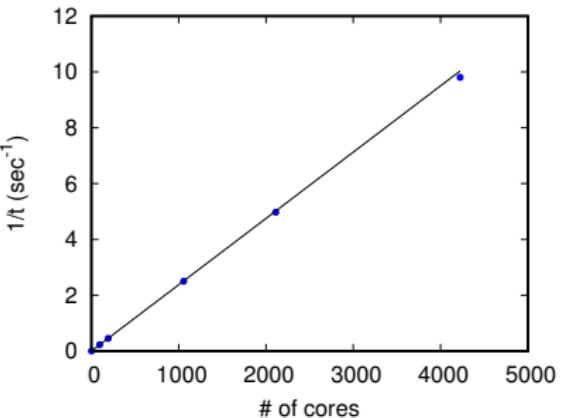
# Scaling

- 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.

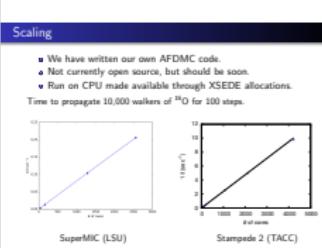


SuperMIC (LSU)



Stampede 2 (TACC)

- Before talking about the wave function let's talk about the scaling of the code.



# 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.

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

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

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

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

# 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.

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

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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.

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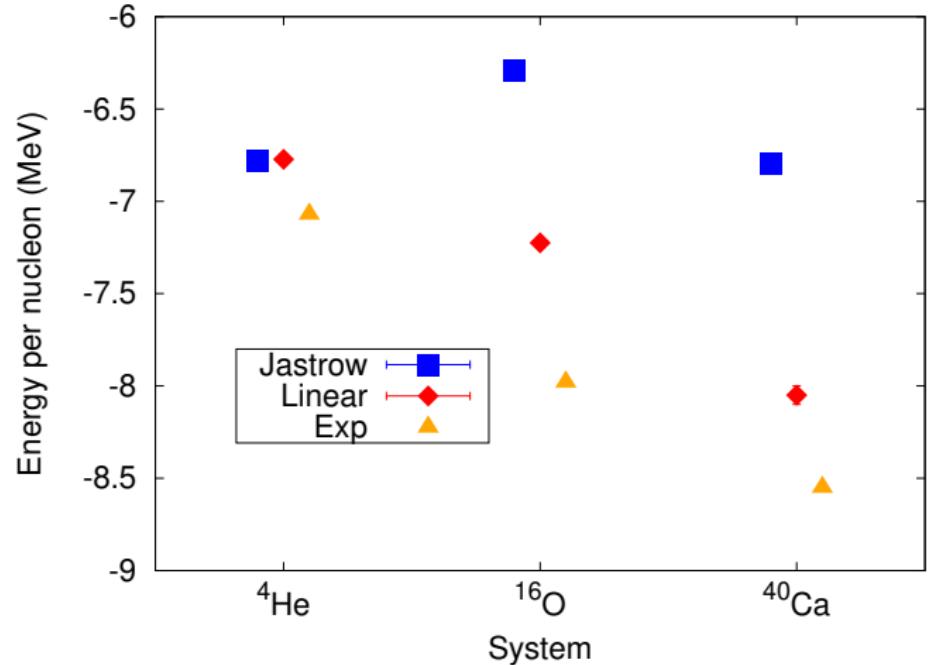
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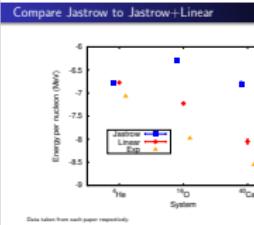
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## Compare Jastrow to Jastrow+Linear



Data taken from each paper respectively.

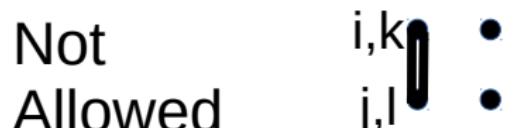
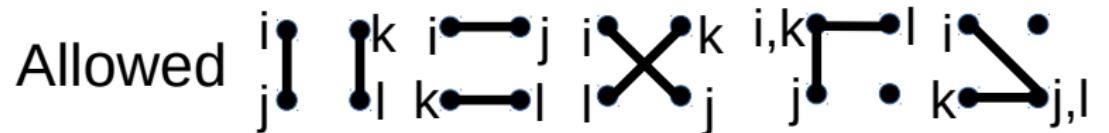


Compare Jastrow to Jastrow+Linear  
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# Symmetrized Product Wave Function

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

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



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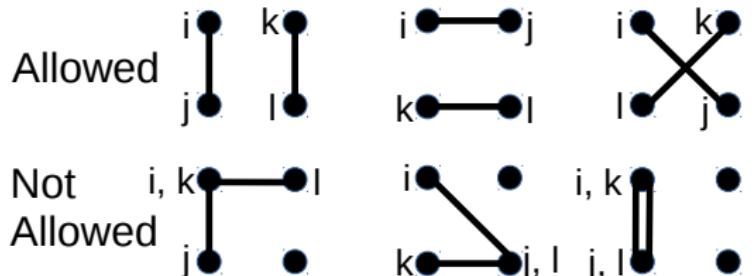
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# Independent Pair Quadratic Correlations

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

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



Or it can be expanded to get independent pair quadratic terms

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



- No need for an explicit symmetrization.

# 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.

2019-05-21

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## Results - AFDMC

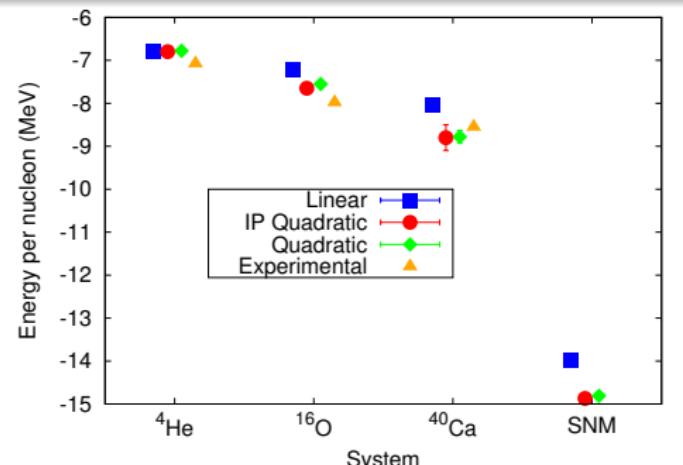
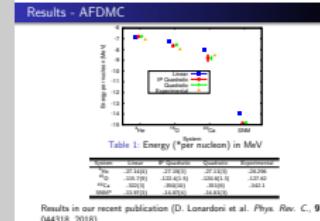


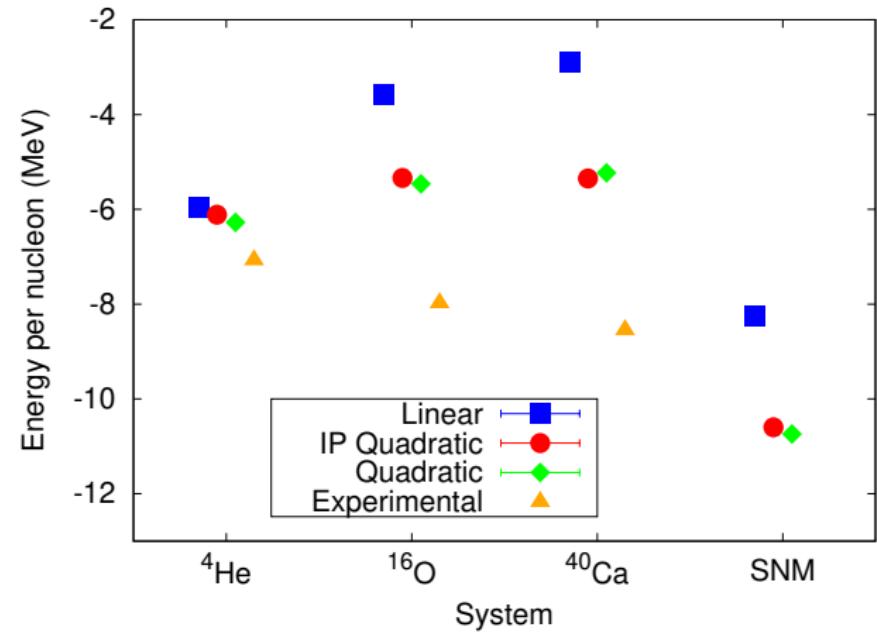
Table 1: Energy (\*per nucleon) in MeV

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)	

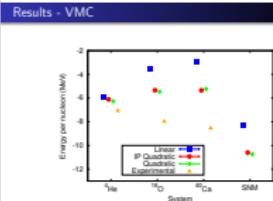
Results in our recent publication (D. Lonardoni et al. *Phys. Rev. C.*, **97**, 044318, 2018).



# Results - VMC



2019-05-21



- Sanity check since AFDMC doesn't have upper bound constraint like VMC.
- ALL decreased in energy, even  $^4\text{He}$ .

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

Calculation	Correlations	<sup>4</sup> He	<sup>16</sup> 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)

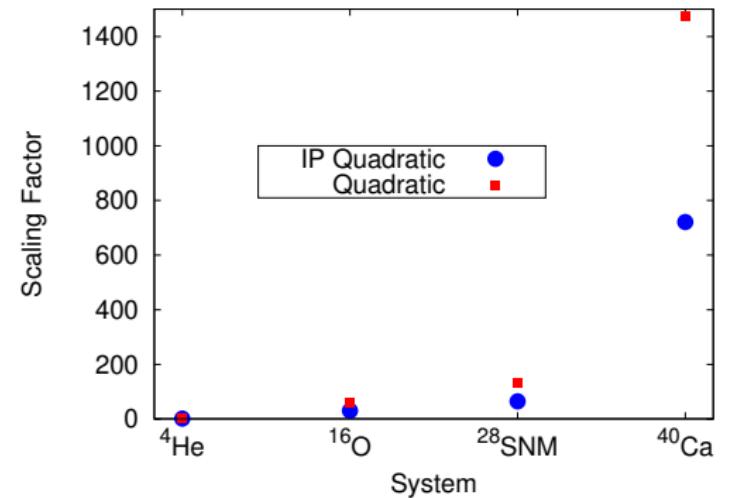
Note that the NN part of N<sup>2</sup>LO includes the spin-orbit interaction, which is not included in AV6' and which has been shown to decrease binding (S. Gandolfi et al. *Phys. Rev. C*, **90**, 061306(R), 2014.).

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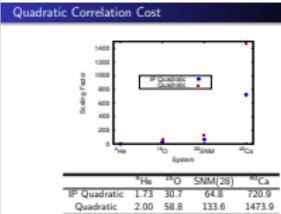
- N<sup>2</sup>LO with  $R_0 = 1$  fm cutoff.
- All the energies are per particle, in MeV.
- All the wave functions have both two- and three-body correlations.
- Local chiral potential at N<sup>2</sup>LO for R0=1.0fm cutoff.
- <sup>4</sup>He and SNM are done with the E1 parametrization.
- <sup>16</sup>O is done with the Etau parametrization.
- <sup>4</sup>He and <sup>16</sup>O also contain the Coulomb.
- Re-optimized for <sup>4</sup>He and <sup>16</sup>O with quadratic.
- No re-optimization for SNM and only used growth energy.
- SNM with no correction for finite size effects.
- All DMC with constrained-path, no transient/unconstrained.

## 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

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- We have a good wave function now, but we still need something that is more efficient.

# 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.

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

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# Exponential Correlations - Preliminary

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

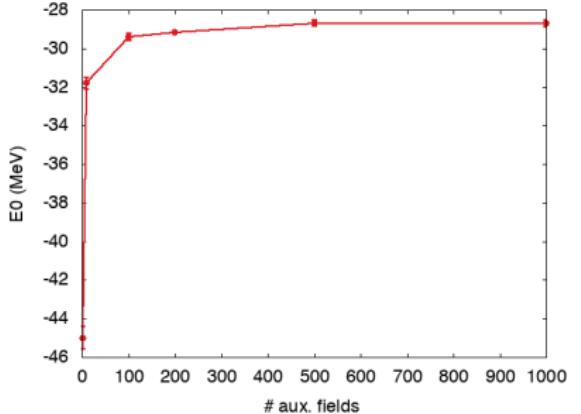


Table 2:  ${}^4\text{He}$  energy with exp correlations.  $E_{\text{linear}} = -26.48(9)$  MeV.

# 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!

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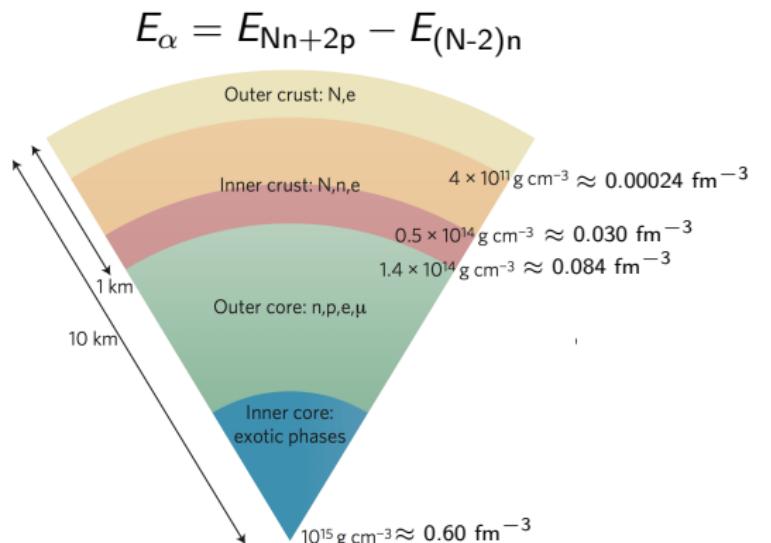
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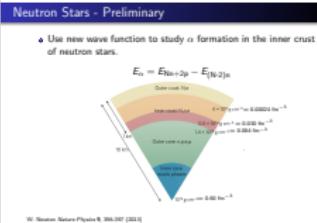
▼ Possible future project!

## Neutron Stars - Preliminary

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



W. Newton *Nature Physics* **9**, 396-397 (2013)



## 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

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

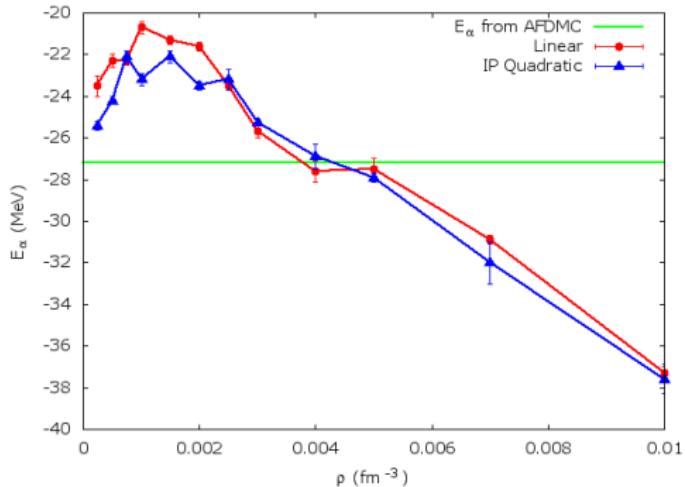
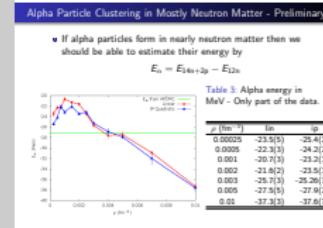


Table 3: Alpha energy in MeV - Only part of the data.

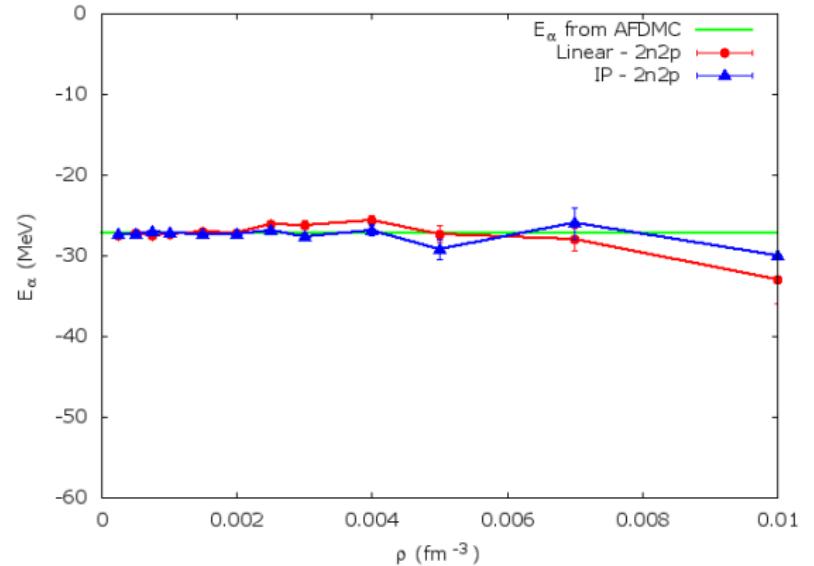
$\rho$ ( $\text{fm}^{-3}$ )	lin	ip
0.00025	-23.5(5)	-25.4(2)
0.0005	-22.3(3)	-24.2(2)
0.001	-20.7(3)	-23.2(3)
0.002	-21.6(2)	-23.5(3)
0.003	-25.7(3)	-25.26(18)
0.005	-27.5(5)	-27.9(2)
0.01	-37.3(3)	-37.6(7)

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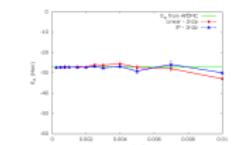
- Green line is what would be expected for an  $\alpha$  alone (see next slide for  $\alpha$  alone).
- Dissolution at about 0.0025 is about what we would expect from other papers.

## 2 Protons + 2 Neutrons Only



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

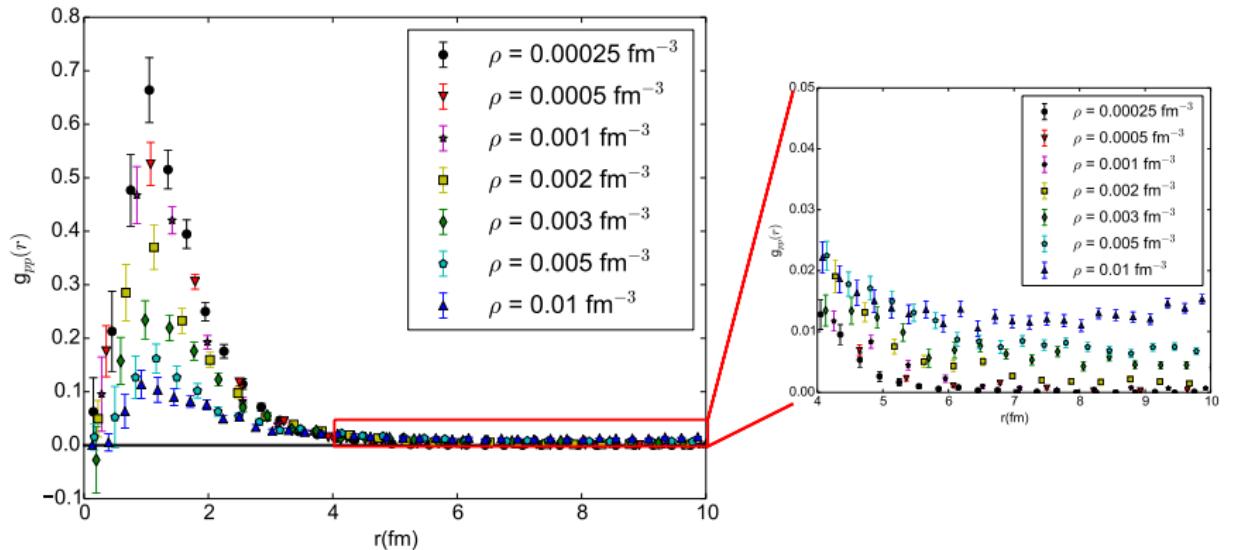
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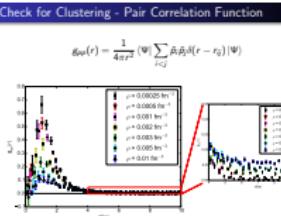
The remaining energy could be due to the  $\alpha$  interacting with the excess neutrons.

## Check for Clustering - Pair Correlation Function

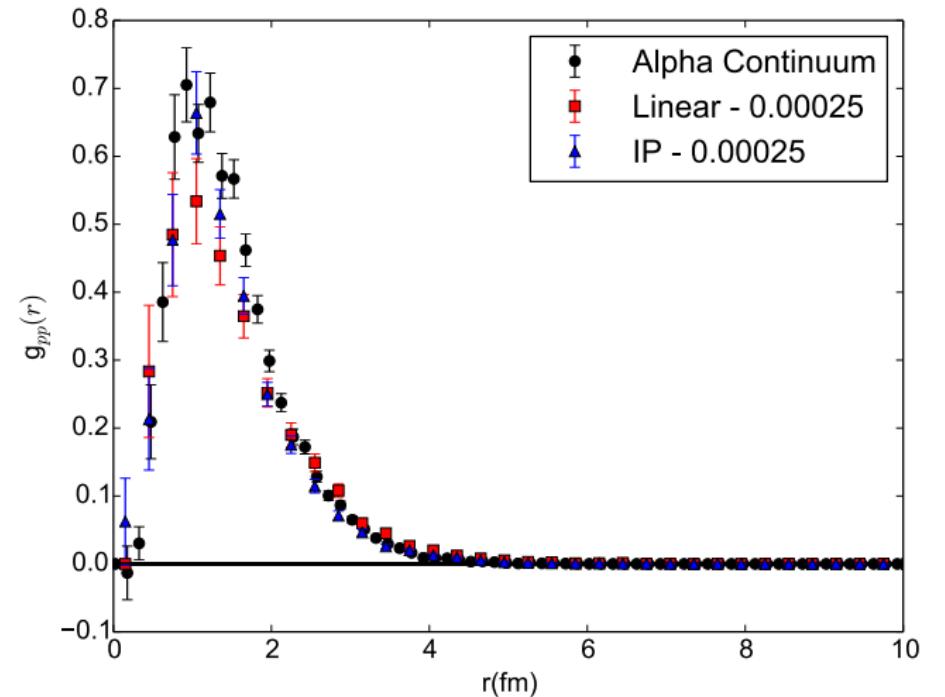
$$g_{pp}(r) = \frac{1}{4\pi r^2} \langle \Psi | \sum_{i < j} \hat{p}_i \hat{p}_j \delta(r - r_{ij}) | \Psi \rangle$$



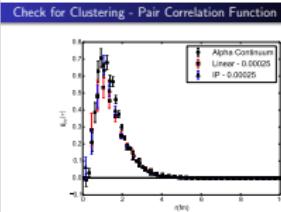
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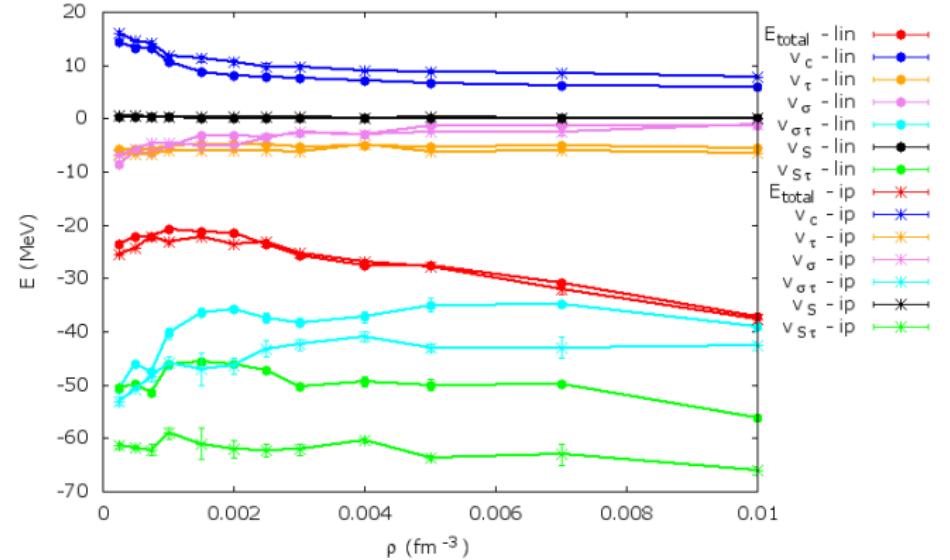


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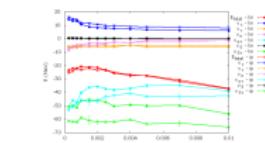
- There is an indication that the IP correlations are forming the  $\alpha$  better than the linear correlations.

## Clustering - Other Insights



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

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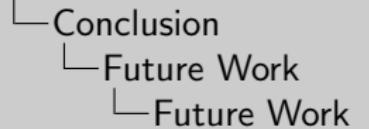


The tensor-tau and sigma-tau (from One Pion Exchange) are most affected by improved correlations.

- This is for the 14n2p calculation at 0.00025 (I think).
- Terms that supplied most binding were most affected by the improved correlations.
- This holds true for other systems as well i.e. 16O.

# 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.



2019-05-21

- 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

Motivation  
Research  
Conclusion

Future Work  
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.

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Conclusion  
└ Conclusion  
  └ Conclusion  
    └ Conclusion

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  - It appears that, at least at low density, the improved wave function correlations are important.

# Thank You

**Advisor:** Kevin Schmidt

**Collaborators:** Stefano Gandolfi (LANL), Joe Carlson (LANL),  
and Diego Lonardoni (MSU-FRIB and LANL), Lucas Madeira  
(ASU and IFSC/USP), Rong Chen (ASU)

**Committee:** Igor Shovkovy, Oliver Beckstein, Ricardo Alarcón



└ Thank You

└ Extra Slides

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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

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

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# 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.

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Two conditions to have convergence to the correct distribution. 1: The steps must be able to get from any allowed state to any other in a finite amount of steps. 2: There cannot be cycles (ACBACBACB...), rejecting some steps gets rid of cycles.

# $\chi$ 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)
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# $\chi$ 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)	—
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# Exponential Correlations - Problems

2019-05-21

## └ 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.

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

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# Exponential Correlations - Problems

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## └ Exponential Correlations - Problems

- Just Almost like before

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

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$$\begin{aligned} \exp \left( \sum_{i < j, p} f_p(r_{ij}) \mathcal{O}_{ij}^p \right) &= \exp \left( \frac{1}{2} \sum_{k\delta=1}^{3A} (\mathcal{O}_{k\delta}^\sigma)^2 \right. \\ &\quad \left. + \frac{1}{2} \sum_{\gamma=1}^3 \sum_{k\delta=1}^{3A} (\mathcal{O}_{k\delta,\gamma}^{\sigma\tau})^2 + \frac{1}{2} \sum_{\gamma=1}^3 \sum_{k=1}^A (\mathcal{O}_{k,\gamma}^\tau)^2 \right) \\ \mathcal{O}_{k\delta}^\sigma &= \sum_{i\alpha} \sum_n \sigma_{i\alpha} \psi_{n,i\alpha}^\sigma (\lambda_n^\sigma)^{1/2} \psi_{n,k\delta}^\sigma \\ \mathcal{O}_{k\delta,\gamma}^{\sigma\tau} &= \sum_{i\alpha} \sum_n \tau_{i\gamma} \sigma_{i\alpha} \psi_{n,i\alpha}^{\sigma\tau} (\lambda_n^{\sigma\tau})^{1/2} \psi_{n,k\delta}^{\sigma\tau} \\ \mathcal{O}_{k\delta}^\tau &= \sum_i \sum_n \tau_{i\gamma} \psi_{n,i}^\tau (\lambda_n^\tau)^{1/2} \psi_{n,k\delta}^\tau \end{aligned}$$

# Exponential Correlations - Problems

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## └ Exponential Correlations - Problems

# Two-Body Operator Updates

2019-05-21

## └ 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.

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This is for an uncorrelated Slater Determinant.

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

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## Two-Body Operator Updates

# 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

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

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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

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## Two-Body Operator Updates

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

# Two-Body Operator Updates - Scaling

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↳ Two-Body Operator Updates - Scaling

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# Forward Walking

- Mixed estimators contain bias from  $\Psi_T$

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

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

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

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$$= \frac{\sum_i \mathcal{O}_i W_i}{\sum_i W_i}$$

$i$  are the random samples (walkers).

## Forward Walking

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EXPLAIN HOW THE PARAMETARS ARE VARIED IN VMC.

Start with basics and then really try to understand it.

See thesis from Casula, New QMC approaches for the simulation  
of electronic systems: a first application to aromatic molecules and  
transition metal compounds.

## └ VMC - Parameter Variation

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Start with basics and then really try to understand it.  
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FINISH THIS! Maybe call it the BCS wave function, which we calculate as a pfaffian of paired orbitals.

2019-05-21

## └ Pfaffian Wave Function

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

# Tensor Force

Slide talking about the physical significance of the tensor force.

## └ Tensor Force

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

## └ Alpha Clusters

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