

# 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

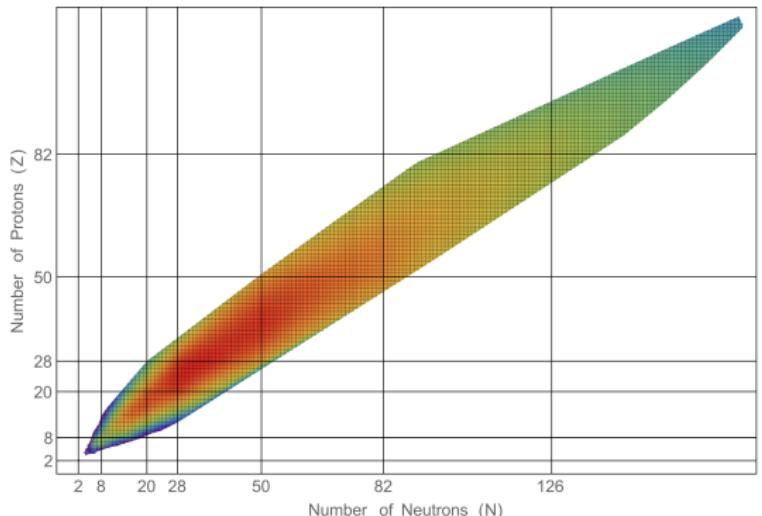
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## └ Outline

# Nuclear Many Body Problem

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

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



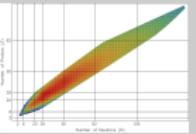
└ Motivation

└ 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.

# Nuclear Many Body Methods

└ Motivation

└ Nuclear Many Body Methods

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- 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

- HF and basis set methods can only use “soft” potentials, but can do non-local potentials.
- QMC complements those because it can do “hard” potentials, but can’t do non-local potentials.

- ▼ There are a number of ways to solve this problem.
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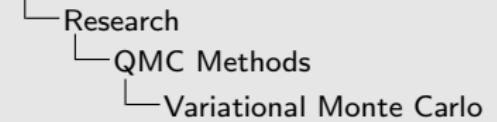
# Variational Monte Carlo

- 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

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

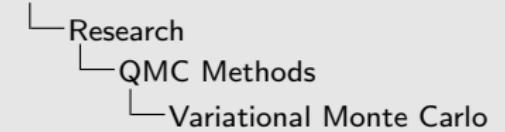
- Multiply and divide the numerator by  $\Psi_T^*(\mathbf{R})\Psi_T(\mathbf{R})$ .

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

- 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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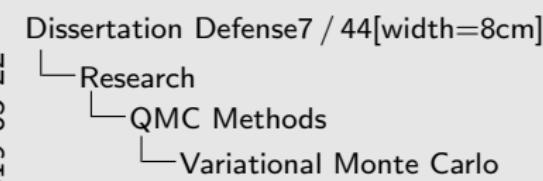
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## Variational Monte Carlo

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- 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.

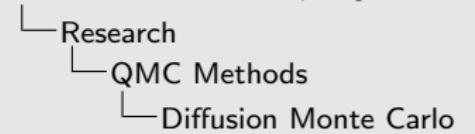
$$H\Psi = i\hbar \frac{d\Psi}{dt} \xrightarrow{\tau=it/\hbar} H\Psi = -\frac{d\Psi}{d\tau}$$

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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## Diffusion Monte Carlo

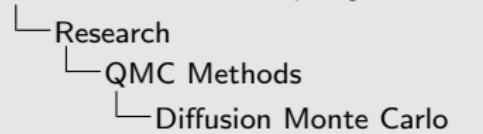
- The propagated wave function can be written

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

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

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

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



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- In practice: Green's function (propagator).
- Can't do full time propagation.
- Can do short time propagation.
- Trotter breakup because of the non-localness of the kinetic energy.
- 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.

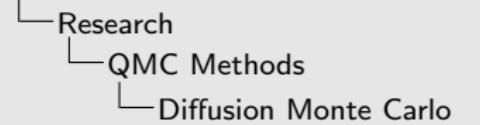
$$\langle \mathbf{R}' | e^{-T\Delta\tau} | \mathbf{R} \rangle = \left( \frac{m}{2\pi\hbar^2\Delta\tau} \right)^{3A/2} e^{-m(\mathbf{R}'-\mathbf{R})^2/2\hbar^2\Delta\tau}$$

- 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

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



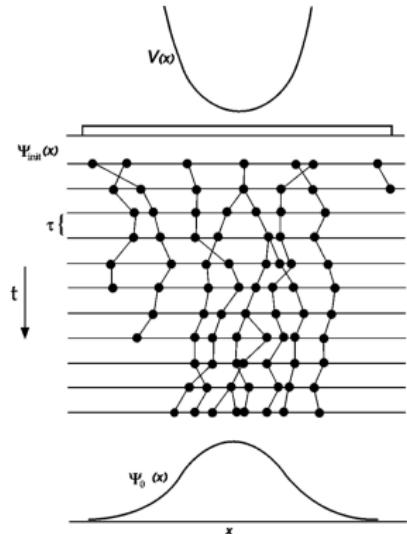
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# Diffusion Monte Carlo - Branching

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.

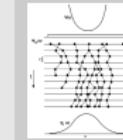


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# Estimating Expectation Values

We want to solve something like this

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

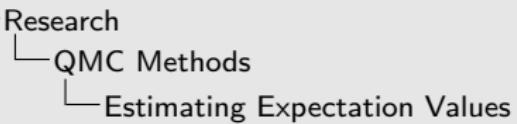
In practice a linear extrapolation is used because  $\mathcal{O}\Psi(\tau)$  is hard.

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

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

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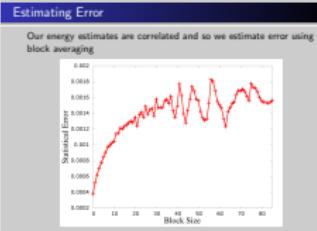
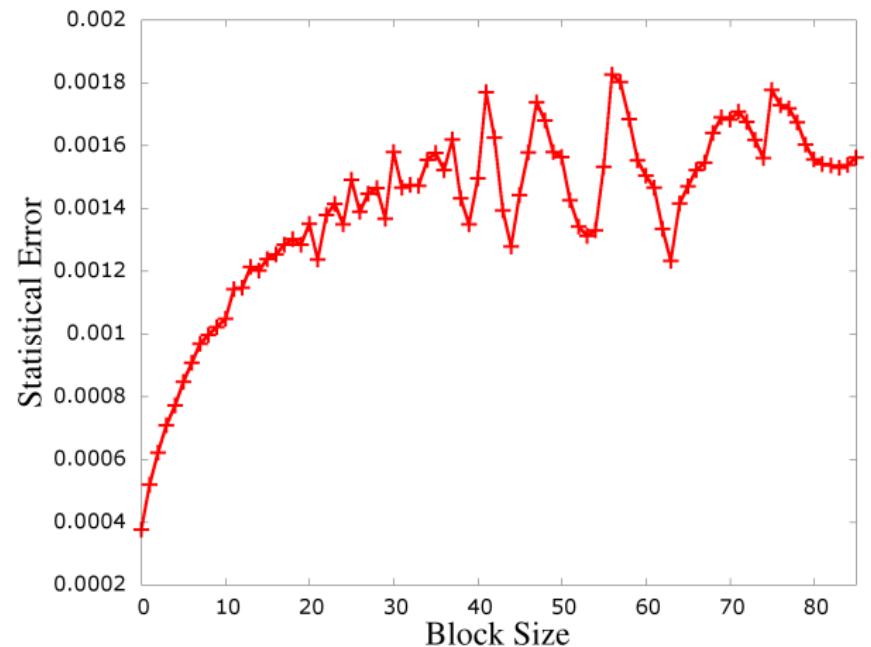
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- START BY SAYING that we use mixed exp to calculate exp values.
- It's difficult to operate through the propagator.
- Accurate to  $\mathcal{O}[(\psi(\tau) - \psi_T)^2]$
- This could be done with **forward walking** but it typically isn't necessary.

# Estimating Error

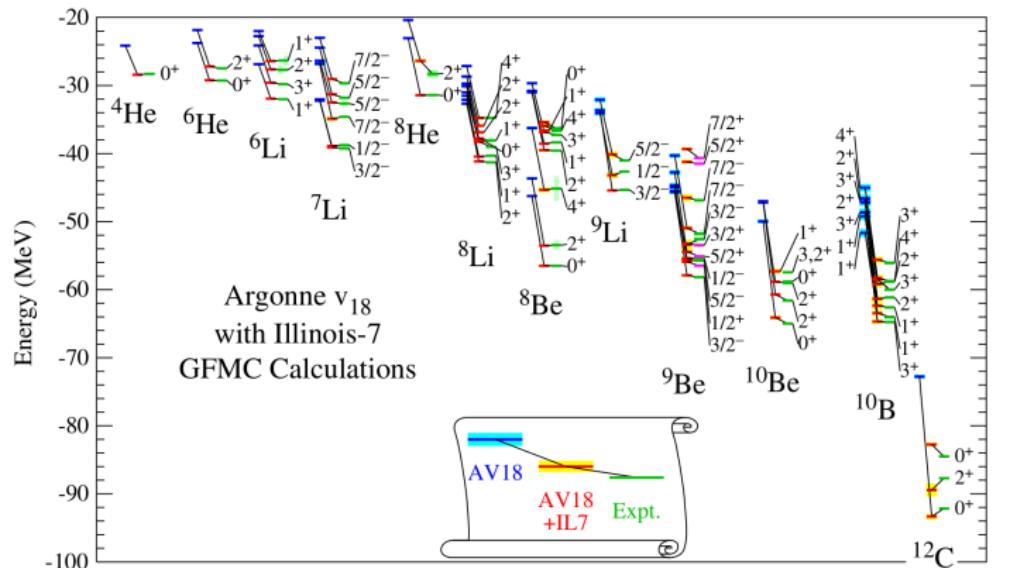
Our energy estimates are correlated and so we estimate error using block averaging



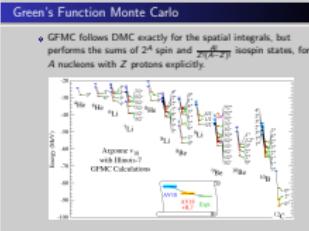
- We don't usually (though you could) talk about the uncertainty in the statistical errors. It's the wiggles at the plateau. We just report 1 digit.

# 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

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

is sampled by using the Hubbard-Stratanovich transformation.

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



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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

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

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

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

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

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# Auxiliary Field Diffusion Monte Carlo - Spin Sampling

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

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

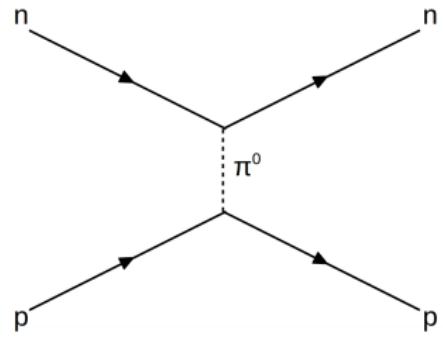
- We have 15A operators (3A for  $O_n^\sigma$ , 9A for  $O_{n\alpha}^{\sigma\tau}$ , and 3A for  $O_{n\alpha}^\tau$ ), the spin-isospin dependent part of the propagator becomes

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

Auxiliary Field Diffusion Monte Carlo - Spin Sampling

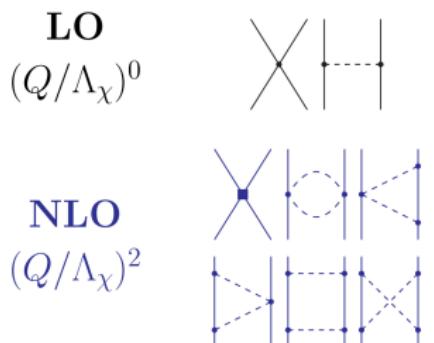
- We have squared single particle operators in the propagator we can now rewrite the propagator in terms of the Hubbard-Stratanovich transformation.
$$e^{-\frac{1}{2}\lambda O^2} = \frac{1}{\sqrt{2\pi}} \int dx e^{-\frac{x^2}{2} + \sqrt{-\lambda}xO}$$
- We have 15A operators (3A for  $O_n^\sigma$ , 9A 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



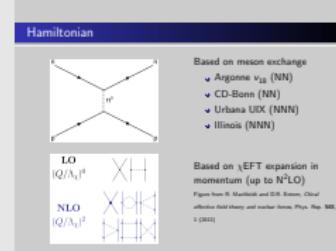
Based on meson exchange

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



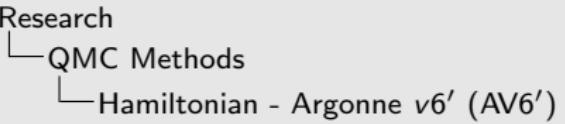
Based on  $\chi$ EFT expansion in momentum (up to  $N^2LO$ )

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



## Hamiltonian - Argonne v6' (AV6')

2019-05-22



- 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

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

$$\begin{aligned}\mathcal{O}_{ij}^0 &= 1, \quad \tau_i \cdot \tau_j, \quad \sigma_i \cdot \sigma_j, \quad \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j, \quad S_{ij}, \quad S_{ij} \tau_i \cdot \tau_j \\ S_{ij} &= 3\sigma_i \cdot \hat{r}_{ij} \sigma_j \cdot \hat{r}_{ij} - \sigma_i \cdot \sigma_j\end{aligned}$$

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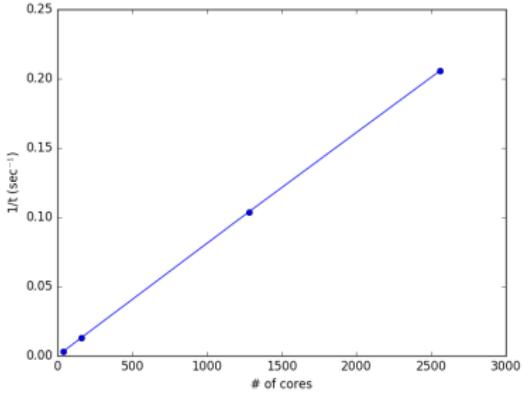
$$\mathcal{O}_{ij}^p = 1, \quad \tau_i \cdot \tau_j, \quad \sigma_i \cdot \sigma_j, \quad \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j, \quad S_{ij}, \quad S_{ij} \tau_i \cdot \tau_j$$

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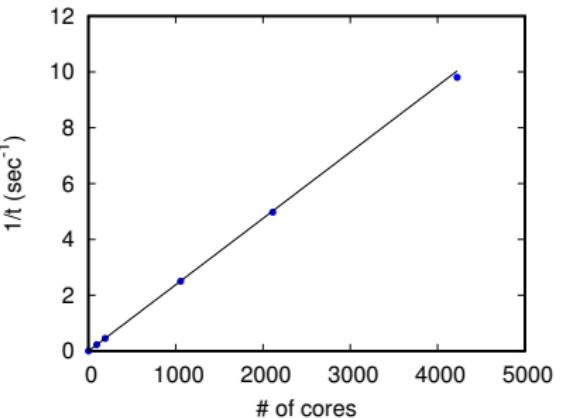
# Scaling

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

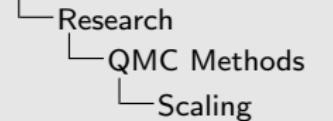
Time to propagate 10,000 walkers of  $^{16}\text{O}$  for 100 steps.



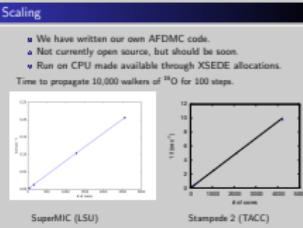
SuperMIC (LSU)



Stampede 2 (TACC)



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

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

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

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## 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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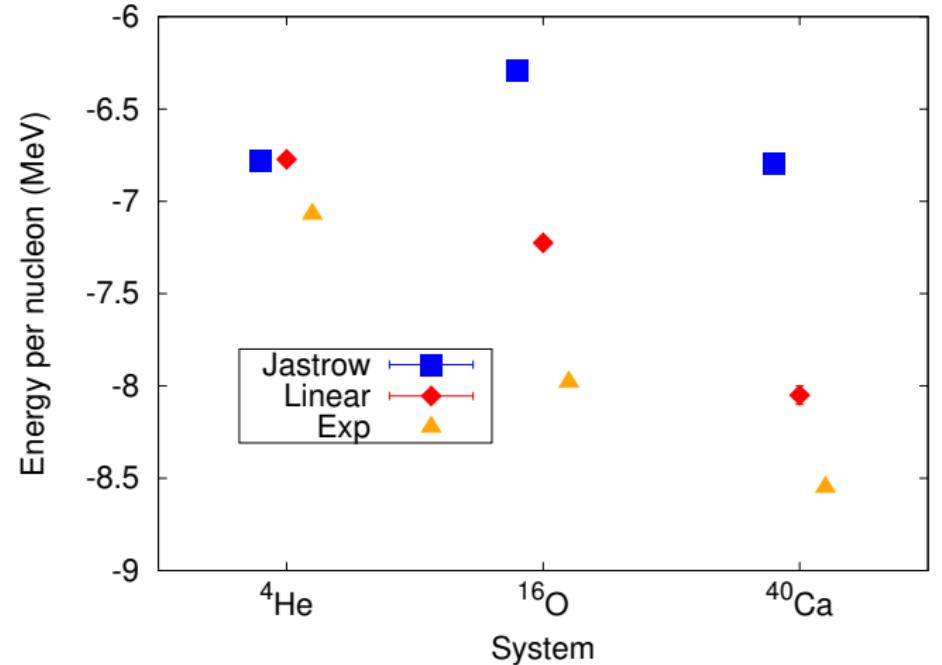
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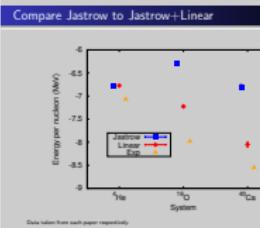
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## Compare Jastrow to Jastrow+Linear



Data taken from each paper respectively.

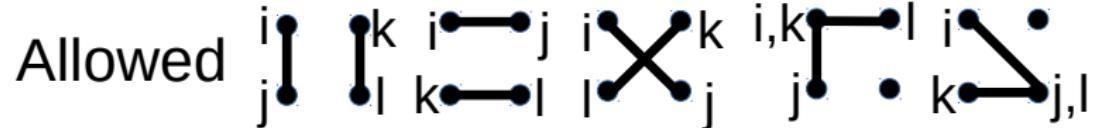


Compare Jastrow to Jastrow+Linear

# Symmetrized Product Wave Function

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

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



Symmetrized Product Wave Function

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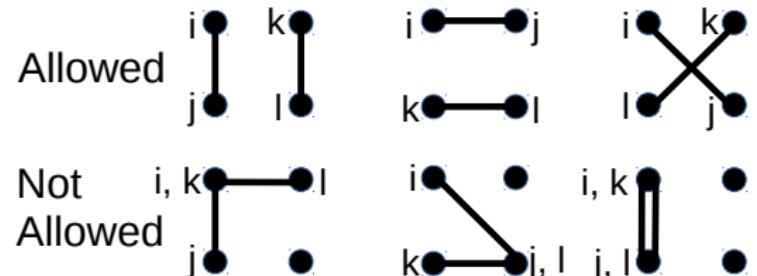
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Allowed						
Not Allowed						

## Independent Pair Quadratic Correlations

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

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**Allowed:**

**Not Allowed:**

# Quadratic Correlations Implementation

Research

Trial Wave Function

Quadratic Correlations Implementation

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- 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

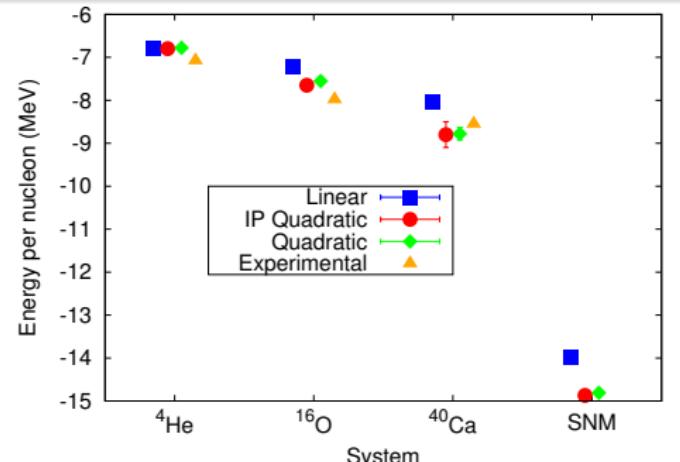
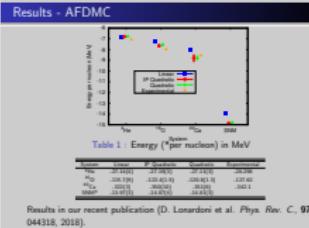


Table 1 : Energy (\*per nucleon) in MeV

System	Linear	IP Quadratic	Quadratic	Experimental
$^4\text{He}$	-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)	

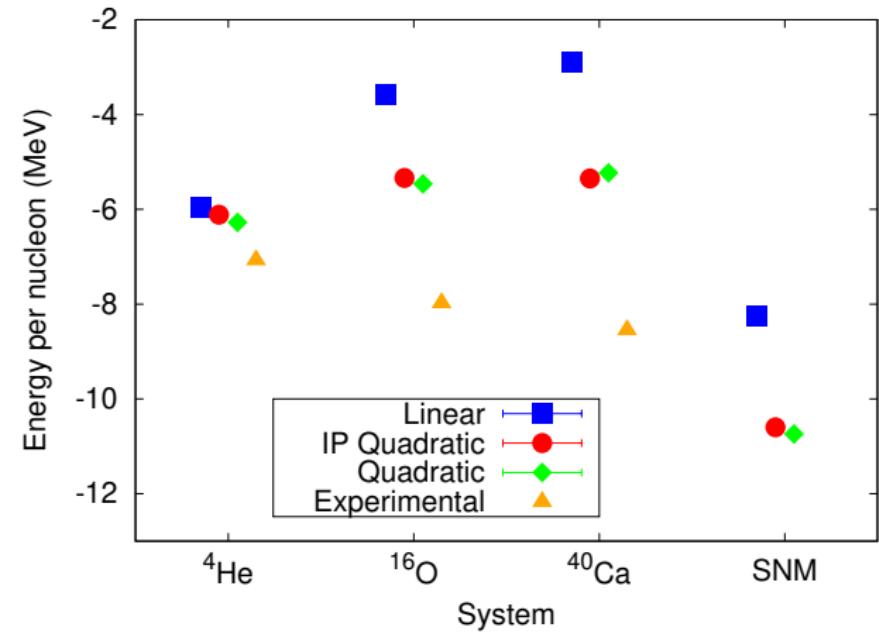
Results in our recent publication (D. Lonardoni et al. *Phys. Rev. C.*, **97**, 044318, 2018).



# Results - VMC

Motivation  
Research  
Conclusion

QMC Methods  
Trial Wave Function  
Alpha Formation in NS

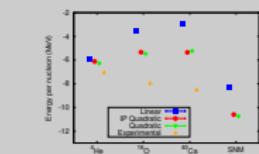


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└ Research  
  └ Trial Wave Function  
    └ Results - VMC

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Results - VMC



- 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)

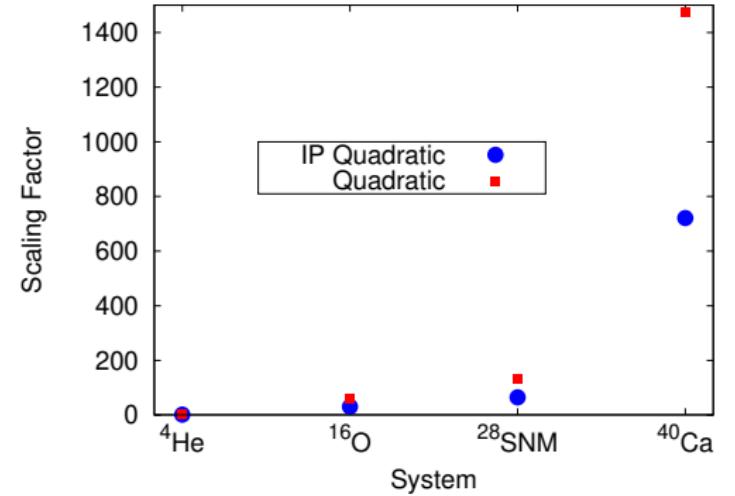
Note that the NN part of N<sup>2</sup>LO includes the spin-orbit interaction, which is not included in AV6' and which has been shown to decrease binding (S. Gandolfi et al. *Phys. Rev. C.*, **90**, 061306(R), 2014.).

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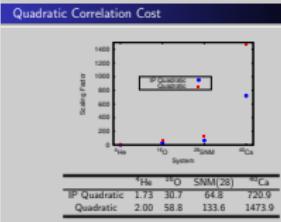
- N<sup>2</sup>LO with  $R_0 = 1$  fm cutoff.
- All the energies are per particle, in MeV.
- All the wave functions have both two- and three-body correlations.
- Local chiral potential at N<sup>2</sup>LO for R0=1.0fm cutoff.
- <sup>4</sup>He and SNM are done with the E1 parametrization.
- <sup>16</sup>O 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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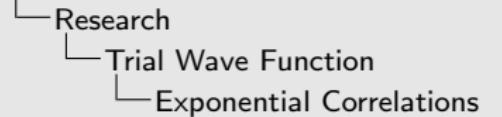
- We have a good wave function now, but we still need something that is more efficient.

# Exponential Correlations

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

- 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.

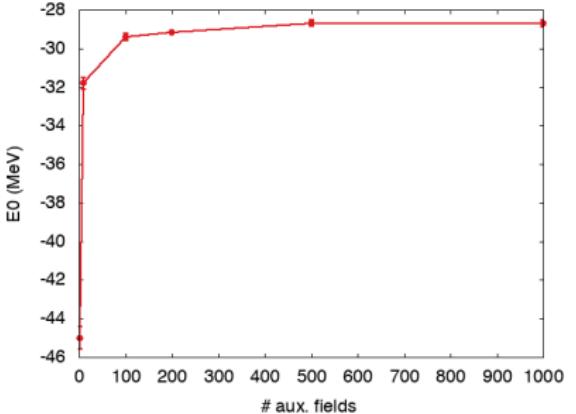
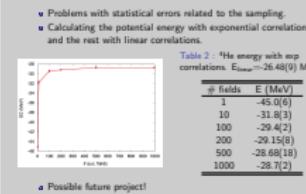


Table 2 :  ${}^4\text{He}$  energy with exp correlations.  $E_{\text{linear}} = -26.48(9)$  MeV.

# 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)

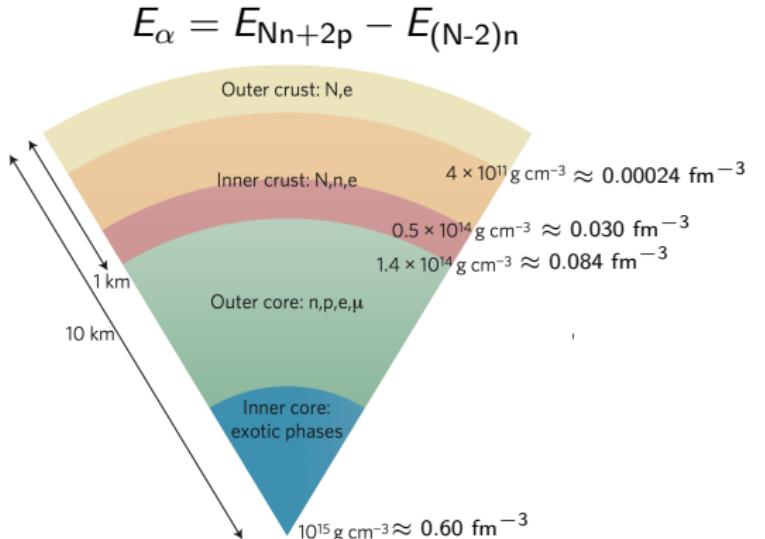
- Possible future project!

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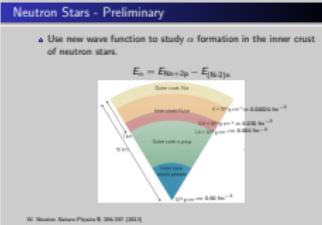


## Neutron Stars - Preliminary

- 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

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

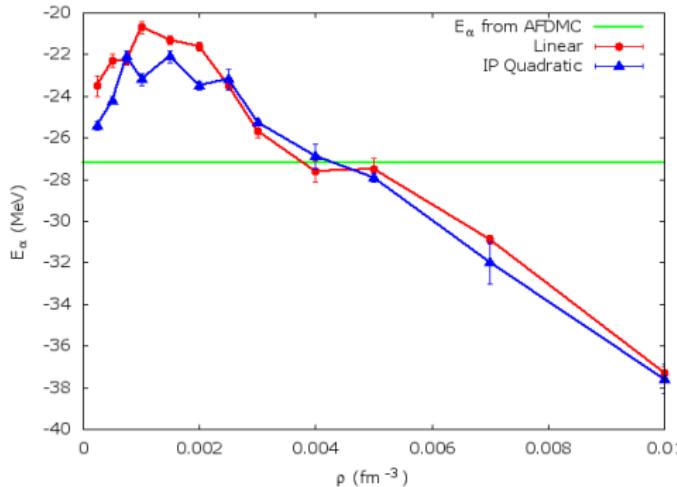
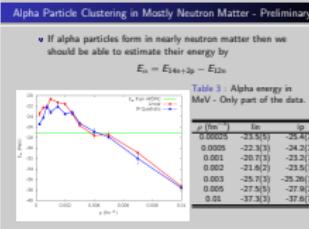


Table 3 : Alpha energy in MeV - Only part of the data.

$\rho$ ( $\text{fm}^{-3}$ )	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)

- 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.



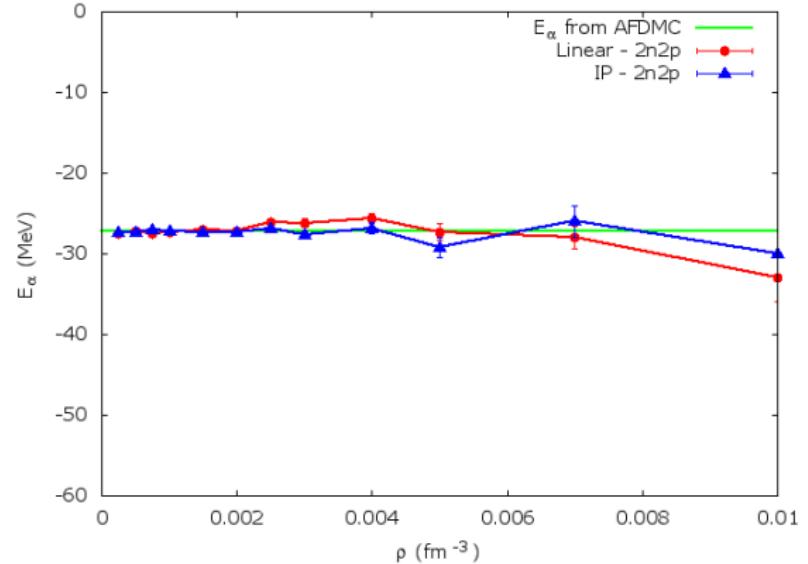
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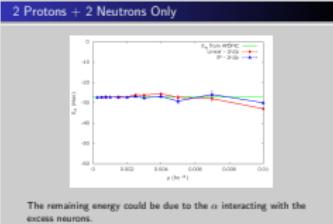
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## 2 Protons + 2 Neutrons Only



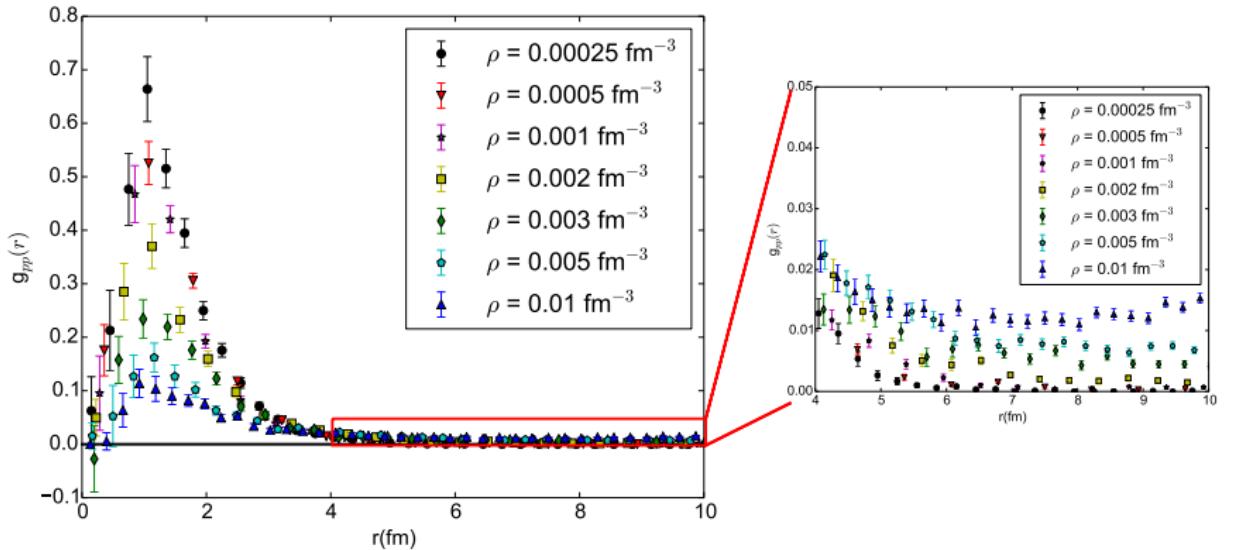
The remaining energy could be due to the  $\alpha$  interacting with the excess neutrons.

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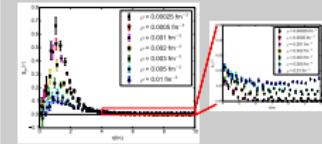
## Check for Clustering - Pair Correlation Function

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

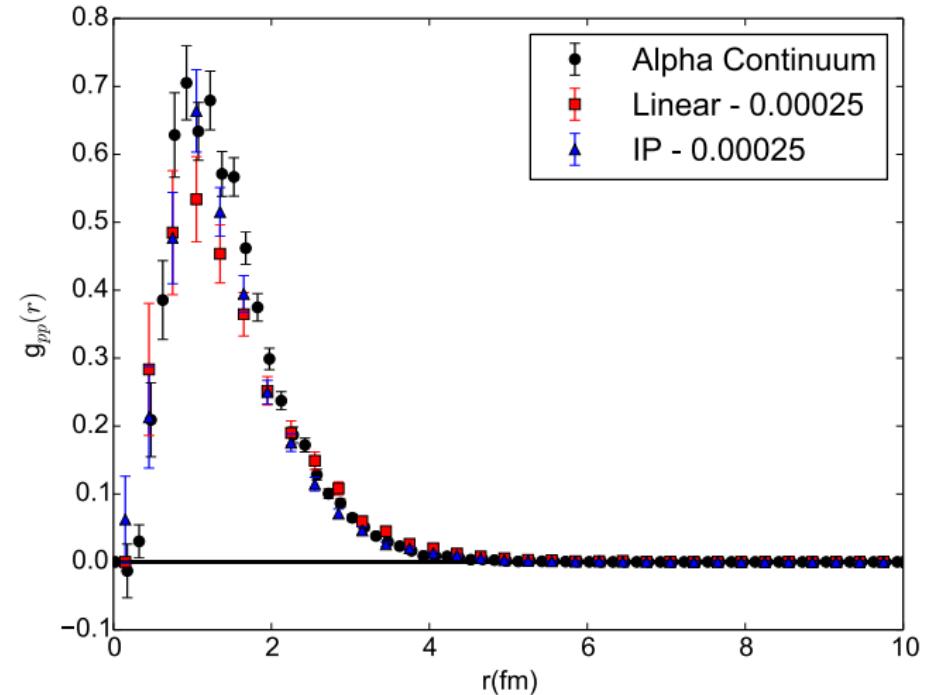


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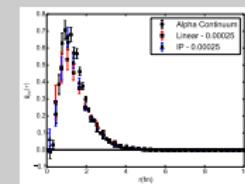
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## Check for Clustering - Pair Correlation Function

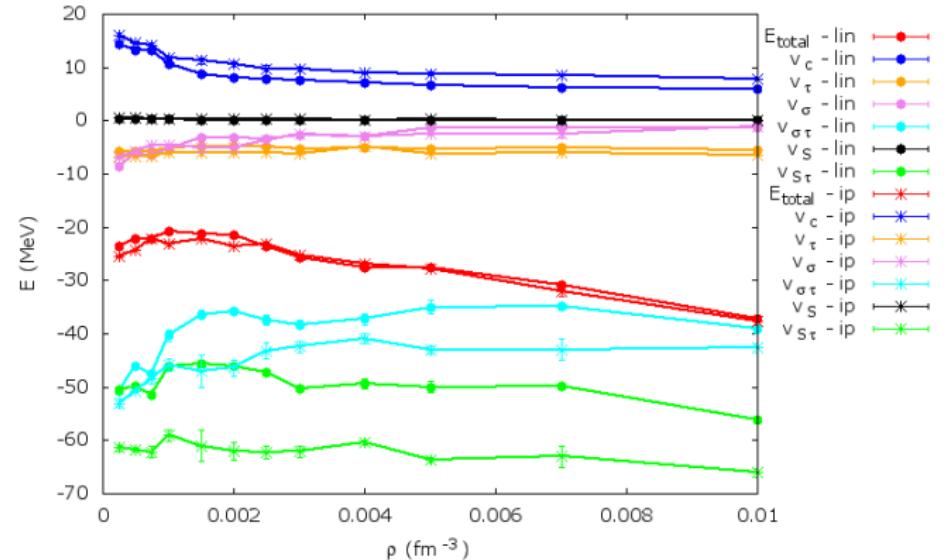


2019-05-22

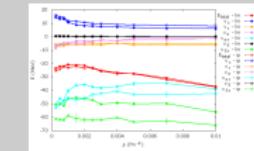


- There is an indication that the IP correlations are forming the  $\alpha$  better than the linear correlations.

## Clustering - Other Insights



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

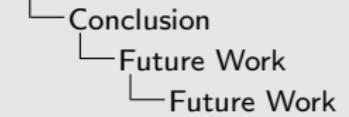


The tensor-tau and sigma-tau (from One Pion Exchange) are most affected by improved correlations.

- 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.



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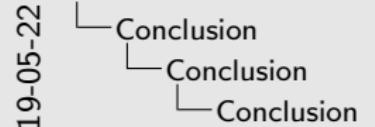
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# Conclusion

Motivation  
Research  
Conclusion

Future Work  
Conclusion

Dissertation Defense 43 / 44 [width=8cm]



2019-05-22

- 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.

Conclusion

- AFDMC calculations need improved correlations for larger systems.
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- 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

**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

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└ Thank You

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# Extra Slides

2019-05-22

└ Extra Slides

# Extra Slides

# Monte Carlo Integration

2019-05-22

## └ 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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# $\chi$ EFT vs. AV6' with AFDMC

2019-05-22

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

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Linear	AV6'	-5.96(1)	-3.581(3)	-8.25(4)
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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

2019-05-22

## └ 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.

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## └ Exponential Correlations - Problems

- Just Almost like before

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

u ~~done~~ Almost like before

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

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## └ Exponential Correlations - Problems

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

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

This is for an uncorrelated Slater Determinant.

2019-05-22

## Two-Body Operator Updates

- $|\chi_{\gamma}\rangle$  are the  $|n \uparrow\rangle$ ,  $|n \downarrow\rangle$ , etc.

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

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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

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# Two-Body Operator Updates

2019-05-22

## 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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# 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

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# Two-Body Operator Updates - Scaling

2019-05-22

## Two-Body Operator Updates - Scaling

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)	$(1 + \mathcal{O}_{ij}^c + \mathcal{O}_{ij}^c \mathcal{O}_{kl}^c) \mathcal{O}_{mn}^p$	$O(A^6)$

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

**Forward Walking**

- Mixed estimators contain bias from  $\Psi_T$ 

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

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## 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

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

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- 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

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## Pfaffian Wave Function

- 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.

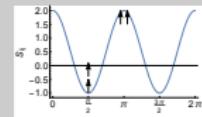
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# Tensor Force

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

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



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