

Oral Comprehensive Exam/Prospectus:  
Improved Trial Wave Function for Quantum Monte  
Carlo Calculations of Nuclear Systems

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March 23, 2017



- $\langle H \rangle = \langle \Psi | H | \Psi \rangle = \int \Psi^*(\mathbf{R}) H \Psi(\mathbf{R}) d\mathbf{R}$
- One of the earliest approximate interactions came from Yukawa<sup>1</sup>.

$$V_Y(r) = -g^2 \frac{e^{-\lambda r}}{r}$$

- The inclusion of NN and NNN terms into this many body Hamiltonian, which could depend on spin and isospin, makes this calculation grow in complexity.

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<sup>1</sup>H. Yukawa. "On the Interaction of Elementary Particles. I.". In: *Proc. Phys. Math. Soc. Japan*. 3rd ser. 17 (1935), p. 48.

- Approximate basis set methods:
  - No-core shell model<sup>2</sup>
  - Coupled-cluster<sup>3</sup>
- Compatibility with local and non-local (velocity dependent) potentials
- Two issues that these methods have
  - Truncation of basis set
  - Poor scaling with basis set size

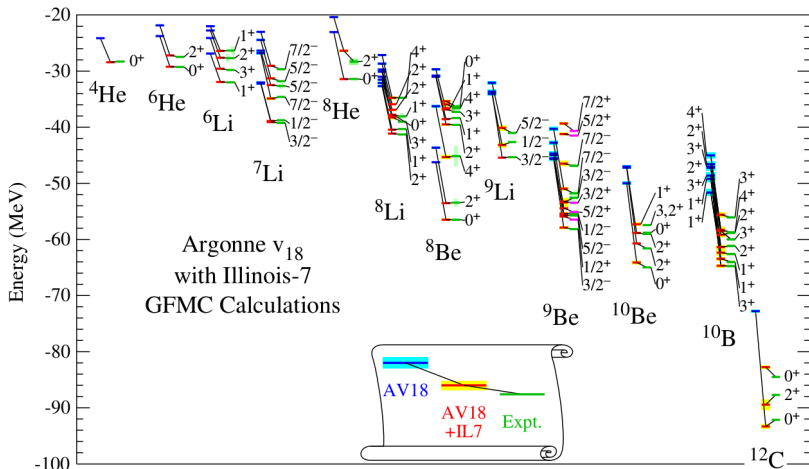
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<sup>2</sup>Bruce R. Barrett, Petr Navrátil, and James P. Vary. “*Ab initio* no core shell model”. In: *Prog. Part. Nucl. Phys.* 69 (2013), pp. 131–181.

<sup>3</sup>G Hagen et al. “Coupled-cluster computations of atomic nuclei”. In: *Rep. Prog. Phys.* 77.9 (2014), p. 096302.

# Background

- GFMC can get results for nuclei up to  $^{12}\text{C}$ .



- We use the phenomenological potential  $AV6'$ , which is a subset of the  $AV18^4$  potential used in GFMC before.

$$v_{ij} = \sum_{p=1,6} v(r_{ij}) \mathcal{O}_{ij}^p$$

$$\mathcal{O}_{ij}^{p=1,6} = 1, \tau_i \cdot \tau_j, \sigma_i \cdot \sigma_j, (\sigma_i \cdot \sigma_j)(\tau_i \cdot \tau_j), S_{ij}, S_{ij}(\tau_i \cdot \tau_j)$$
$$S_{ij} = 3(\sigma_i \cdot \mathbf{r}_{ij})(\sigma_j \cdot \mathbf{r}_{ij}) - \sigma_i \cdot \sigma_j$$

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<sup>4</sup>R.B. Wiringa, V. G. J. Stoks, and R. Schiavilla. "Accurate Nucleon-Nucleon Potential with Charge-Independent Breaking". In: *Phys. Rev. C* 51 (1995), pp. 38–51.

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

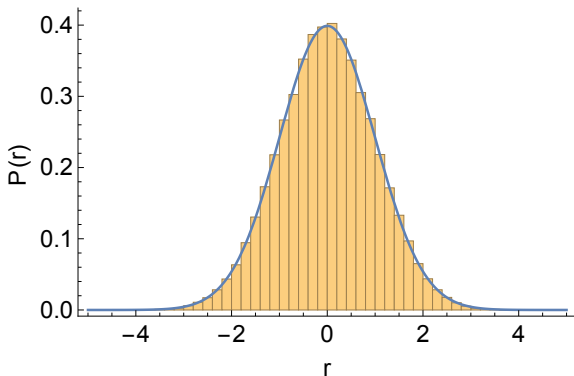
$$I = \int f(\mathbf{R}) P(\mathbf{R}) d\mathbf{R}$$

- 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

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

# Sampling $P(\mathbf{R})$

- We need to draw samples from a probability density. If this is an function with an invertible CDF this is easy to do.



$$r = \text{CDF}^{-1}(\xi)$$

- If not then we need to use other methods to sample the distribution.



# 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  $T$  can be a Gaussian centered on the current position.
- 3 The probability of accepting the move is given by

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

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

# Variational Monte Carlo

- VMC starts with a trial wave function which includes variable parameters.
- The variational principle guarantees

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

- To use what we learned above we want this to look like this

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

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

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

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

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

- 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  $E_V \geq E_0$ .

# Variational Monte Carlo - Implementation

- ① Generate  $N$  configurations (walkers) distributed randomly.
- ② Loop over each walker and do the following
  - ① Calculate  $P(\mathbf{R}) = |\langle \Psi_T | \mathbf{R} \rangle|^2$
  - ② Propose a move  $\mathbf{R}' = \mathbf{R} + \Delta\xi$ , where  $\xi$  could be a vector of random variable from a Gaussian.
  - ③ Calculate  $P(\mathbf{R}') = |\langle \Psi_T | \mathbf{R}' \rangle|^2$
  - ④ Calculate the probability of acceptance  $A = \min\left(1, \frac{P(\mathbf{R}')}{P(\mathbf{R})}\right)$
  - ⑤ If accepted then  $\mathbf{R} \rightarrow \mathbf{R}'$ , else the next position in the Markov Chain for that walker is the same as the last, namely  $\mathbf{R}$
- ③ Calculate observables and repeat steps 2 until energy is minimized or uncertainties are low enough.

- Diffusion Monte Carlo uses a Green's function to diffuse walkers 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.

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

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

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

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

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

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

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

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

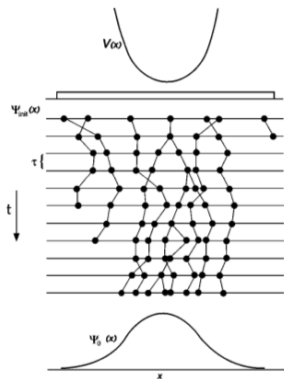
- Importance sampling improves the variance of the sampling and can be included with

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



# Diffusion Monte Carlo

Branching: 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.

# Diffusion Monte Carlo - Implementation

- ① Start with  $N$  configurations (walkers) from VMC
- ② Loop over each walker and do the following
  - ① Propose a move,  $\mathbf{R}' = \mathbf{R} + \chi$ , where  $\chi$  is a random number from the shifted Gaussian  $\exp\left(\frac{m}{2\hbar^2\Delta\tau}\left(\mathbf{R}' - \mathbf{R} + 2\frac{\nabla\Psi_I(\mathbf{R}')}{\Psi_I(\mathbf{R}')}\right)^2\right)$ .
  - ② The move is then accepted with the probability  $A(\mathbf{R}' \leftarrow \mathbf{R}) = \min\left(1, \frac{\Psi_T^2(\mathbf{R}')}{\Psi_T^2(\mathbf{R})}\right)$ .
  - ③ Calculate the weight  $w(\mathbf{R}') = \exp(-(E_L(\mathbf{R}') + E_L(\mathbf{R}) - 2E_0)\Delta\tau/2)$ .
  - ④ Do branching.
  - ⑤ Calculate and collect the observables and uncertainties needed and increase the imaginary time by  $\Delta\tau$ .
- ③ Repeat from step 2 to 6 until the uncertainties are small enough.

# Auxiliary Field Diffusion Monte Carlo - Spin Sampling

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

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

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

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

# Auxiliary Field Diffusion Monte Carlo - Spin Sampling

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

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

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

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

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

$$\sum_j A_{ij}^{\tau} \psi_{n,j}^{\tau} = \lambda_n^{\tau} \psi_{ni}^{\tau}$$

# Auxiliary Field Diffusion Monte Carlo - Spin Sampling

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

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

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

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

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

# Auxiliary Field Diffusion Monte Carlo - Spin Sampling

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

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

- Since 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 dependant part of the propagator becomes

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

- The simplest wave function for a many-fermion system is a Slater determinant.

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

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

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

where  $\langle RS|\phi\rangle$  is the Slater determinant described above.

# Full Trial Wave Function

- A completely cluster decomposable ( $|\Phi_A + \Phi_B\rangle = |\Phi_A\rangle |\Phi_B\rangle$ ) set of spin-isospin dependent correlations could be an exponential

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

- However, a symmetrized product wave function captures almost the same physics.

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



# Quadratic Correlations

- If we assume the correlations are small we can expand this exponential to first order.

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

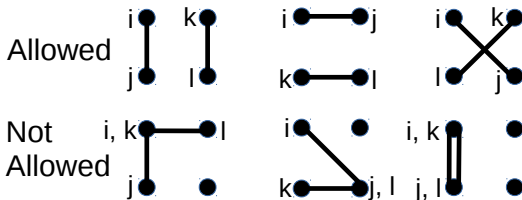
- By expanding the product you can write this as

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

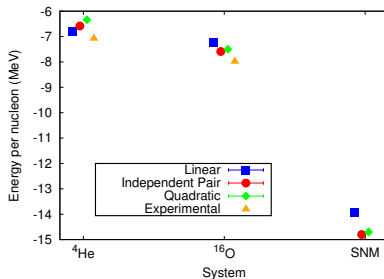
# Independent Pair Correlations

- Or it can be expanded to get independent pair terms

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



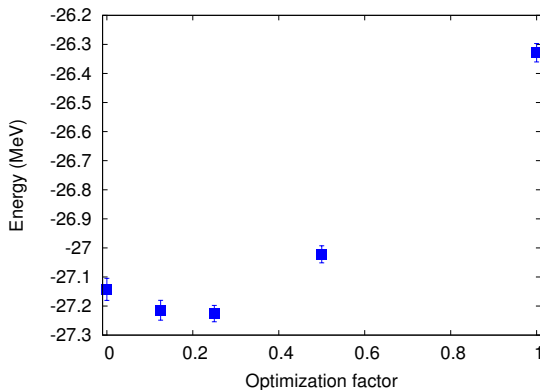
# Results



	Linear	IndPair	Quadratic	Expt.
$^4\text{He}$	-27.17(4)	-26.33(3)	-25.35(3)	-28.295
$^{16}\text{O}$	-115.7(9)	-121.5(1.5)	-120.0(1.4)	-127.619
SNM( $\rho = 0.16 \text{ fm}^{-3}$ )	-13.92(6)	-14.80(7)	-14.70(11)	

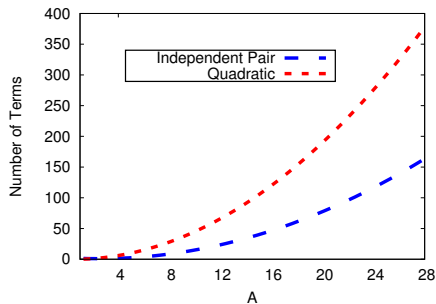
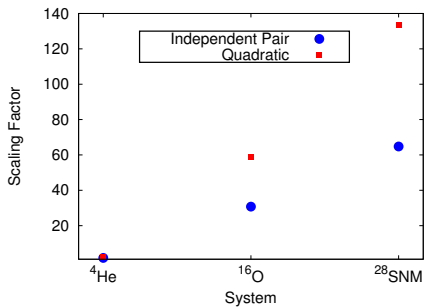
Energies (per nucleon) in MeV, SNM was done with 28 particles with periodic boundary conditions.

# Results



Optimization of quadratic  $\beta$  parameter for  $^4\text{He}$  with independent pair correlations.

# Results



	$^4\text{He}$	$^{16}\text{O}$	$^{28}\text{SNM}$
Independent Pair	1.73	30.7	64.8
Quadratic	2.00	58.8	133.6

- We have added independent pair and full quadratic correlations to the already linearly correlated wave function.
- The addition of these operators decreases the energy for each system.
- Though there was not a large difference between independent pair and full quadratic correlations the scaling was about twice as good for independent pair correlations.

# End of Comprehensive

Questions?

- I will apply these calculations to other medium mass nuclei.
  - $^{40}\text{Ca}$
  - Other isotopes of Oxygen
  - Open shell nuclei
- This work will then be published.
  - Draft by the end of the summer.
- When this project is done I plan to move on to one or more additional projects.



# Exponential Correlations

- Another way to improve the trial wave function is to start with the exponential correlations and use the Hubbard-Stratanovich transformation to sample them, just like we do for the spin-isospin part of the propagator in AFDMC.

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

# Exponential Correlations

- Compare what we have for the potential (without the Jastrow part) to what we have for the Green's function.

$$\langle \psi_T | RS \rangle = \langle \phi | e^{\sum_p \sum_{i < j} f_p(r_{ij}) \mathcal{O}_{ij}^p} | RS \rangle$$

$$G_{SD}(R'S', RS, \Delta\tau) = \langle R'S' | e^{\sum_p \sum_{i < j} u_p(r_{ij}) \mathcal{O}_{ij}^p \Delta\tau} | RS \rangle$$

- The only differences between these are the different function  $u$  and  $f$ , and the  $\Delta\tau$ . Then the correlations in the trial wave function can be written as

$$e^{\sum_p \sum_{i < j} f_p(r_{ij}) \mathcal{O}_{ij}^p} = \prod_{n=1}^{15A} \frac{1}{\sqrt{2\pi}} \int dx_n e^{-\frac{x_n^2}{2}} e^{\sqrt{-\lambda_n} x_n \mathcal{O}_n}.$$

# Exponential Correlations

- To improve the variance of sampling the average of with samples  $x$  and  $-x$  is taken.
- This improved wave function will allow us to study larger nuclear system like neutron-rich nuclei created by the r-process.

# Particle Clustering in Nuclear Matter

- When a nucleus has an even number of  $n$  and  $p$  each  $n$  pairs with a  $p$ , and this decreases the energy of the system.
- However two  $n$  and two  $p$  can pair together to form an  $\alpha$ -particle.
- At low densities quartetting is more energetically favorable than pairing<sup>5</sup>.
- I want to show that we can see this clustering.
- I also want to do calculations at different densities to study how these clusters dissolve as a function of density.

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<sup>5</sup>P. Schuck et al. "Alpha-Particle Condensation in Nuclear Systems". In: *J. Phys.: Conf. Ser.* 413 (2013), p. 012009.

# Neutron Star

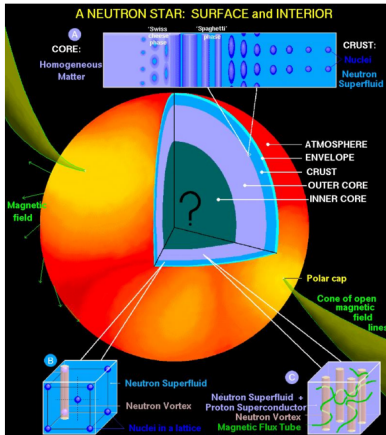


Figure: Reprinted from  
Dany Page et al. *Annu.  
Rev. Nucl. Part. Sci.*,  
56:327-374, 2006.

# Particle Clustering in Nuclear Matter

- Calculate the energy/particle ( $E_{14n}/14$ ) of pure neutron matter with 14 particles in a periodic box and compare with 14 neutrons plus 2 protons ( $E_{14n2p}/16$ ).
- If there is quartetting there should be a shift in the energy.

$$E_{14n2p}/16 \approx (E_{12n} + E_{\alpha})/16$$

- If neutron matter had energy  $E_n/N \approx 15\text{MeV}$  and the alpha  $E_{\alpha} \approx -28\text{MeV}$  this would be

$$E_{14n2p}/16 \approx \left( 15 \frac{\text{MeV}}{\text{part}} \cdot 12 - 28\text{MeV} \right) / 16 = 4\text{MeV}$$

# Particle Clustering in Nuclear Matter

Here put something about the  $g(r)$  pair distributions

# Timetable

Summer 17	Submit draft for quadratic correlations paper
Fall 17	"Complete" exponential correlations project
Spring 18	"Complete" alpha clustering project
Summer 18	Submit a draft of alpha clustering paper
Fall 18	Start writing dissertation
Spring 19	Finish dissertation and defence



- Current XSEDE Allocation: 100,000 hours on LSU SuperMIC
  - Quadratic Correlations: 100,000 hours
- Future XSEDE Allocation: 480,000 hours on LSU SuperMIC
  - Exponential Correlations: 240,000 hours
  - Alpha Clustering: 240,000 hours

# Dissertation Breakdown

- ① Introduction
- ② Methods
  - ① Variational Monte Carlo
  - ② Diffusion Monte Carlo
  - ③ Auxiliary Field Diffusion Monte Carlo
  - ④ Hamiltonian
- ③ Trial Wave Function
  - ① Expand the Symmetric Product Wave Function
  - ② Exponential Wave Function
  - ③ Comparing Trial Wave Functions
- ④ Alpha Clustering in Nuclear Matter
  - ① Theory
  - ② Results
- ⑤ Conclusion