

# Improved trial wave functions with 4-body correlations for Nuclear Quantum Monte Carlo

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# Outline

- Quantum Monte Carlo methods
- Current trial wave function
- Improved trial wave functions
- Results/Conclusion

# Quantum Monte Carlo

- **VMC:**

$$E_V = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0$$

- **AFDMC:**

$$\Psi_0(\mathbf{R}) = \lim_{\tau \rightarrow \infty} \langle \mathbf{R} | e^{-(H-E_0)\tau} | \Psi_T \rangle$$

- $\Psi_T$  is calculated in practically every part of the calculation and plays an important role in guiding the propagation and diffusion of the calculation to the ground state.

# Slater Determinant

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



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

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



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

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

# Spin Dependent Correlations

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

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

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

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

# Linear Correlations

- Until recently these wave functions had been expanded only to linear order in  $\mathcal{O}_{ij}$ .

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

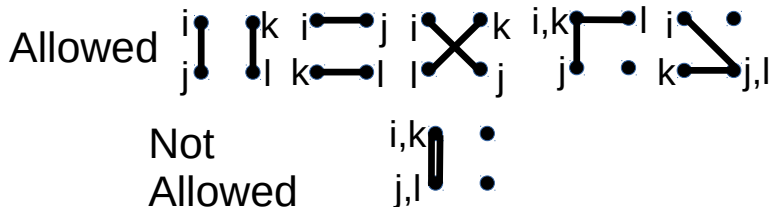
- We have expanded this by including terms up to quadratic order,  $\mathcal{O}_{ij}\mathcal{O}_{kl}$ .



# Quadratic Correlations

- Symmetrized product wave function up to quadratic order

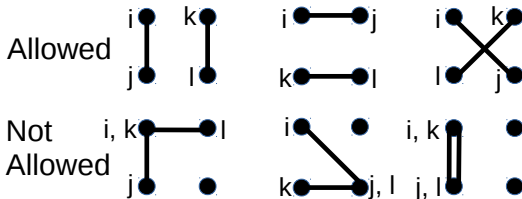
$$|\psi_T\rangle = \left[ \prod_{i<j} f_c(r_{ij}) \right] \left[ 1 + \sum_{i<j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p + \frac{1}{2} \sum_{i<j} \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p \sum_{\substack{k<l \\ ij \neq kl}} \sum_q f_q(r_{kl}) \mathcal{O}_{kl}^q \right] |\phi\rangle$$



# Independent Pair Quadratic Correlations

- Independent pair expansion to quadratic order

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



# Results

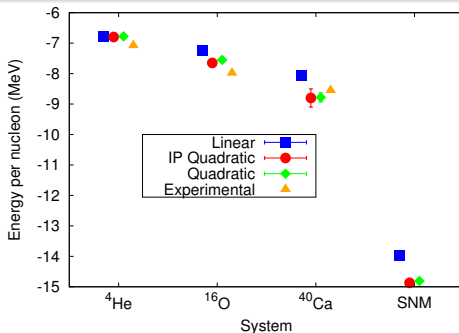
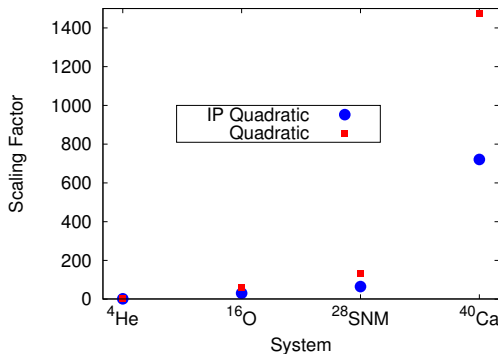


Table: Energy (\*per nucleon) in MeV

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)	

# Quadratic Correlation Cost



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

# Summary/Conclusion

- We have improved the previously used two-body spin-isospin correlations.
- The improved trial wave functions appear to make a significant difference in the energy of the calculations, but currently cost too much to use for large systems.
- AFDMC is a powerful method for solving nuclear many-body problems, however more accurate wave functions are needed to accurately describe larger systems.

# Thanks

Advisor: Kevin Schmidt (ASU)

Collaborators: Stefano Gandolfi (LANL) and Joe Carlson (LANL)



# Extra Slides

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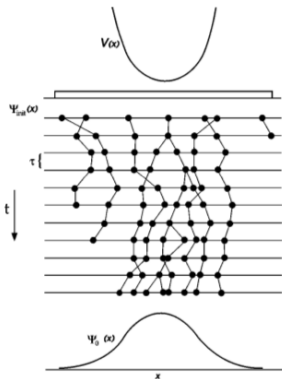
# Variational Monte Carlo - Implementation

- 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 variables 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 - 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.

# Diffusion Monte Carlo - Short Time Propagator

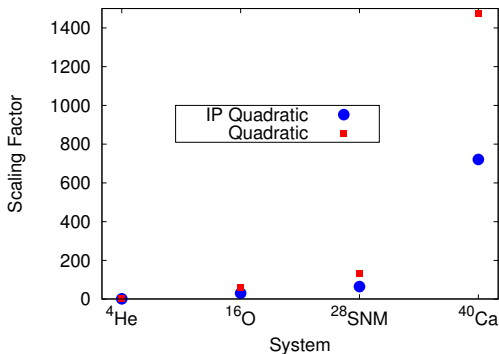
$$\langle \mathbf{R}_N | \Psi_T(\tau) \rangle = \int d\mathbf{R}_1 \dots d\mathbf{R}_N \left[ \prod_{i=1}^N G(\mathbf{R}_i, \mathbf{R}_{i-1}, \Delta\tau) \right] \langle \mathbf{R}_0 | \Psi_T(0) \rangle$$

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

# Diffusion Monte Carlo - 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 vector of random numbers 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.

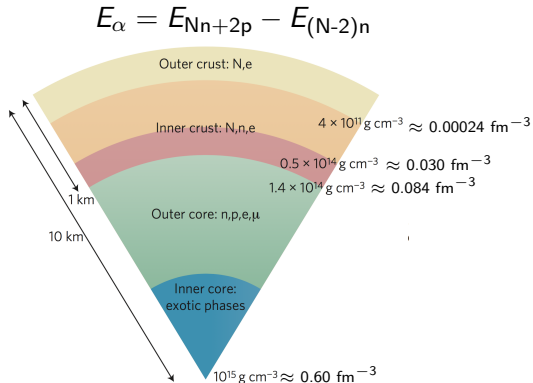
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# Neutron Stars - Preliminary

- 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

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

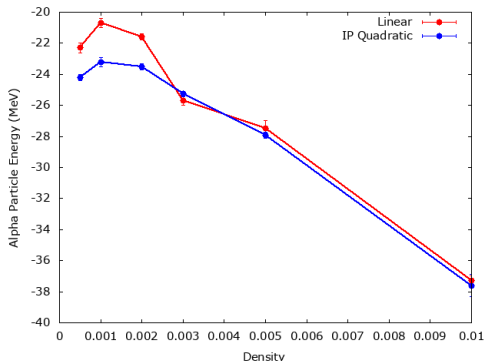
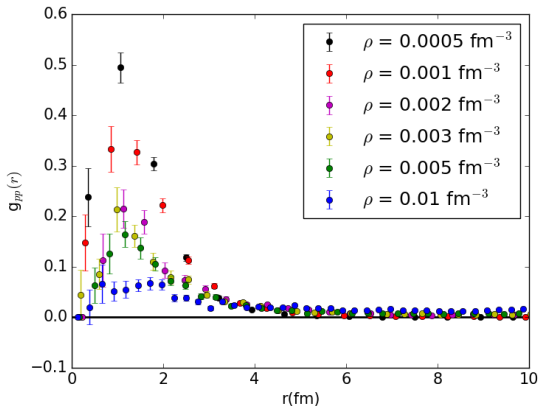


Table: Alpha energy in MeV

$\rho$ (fm <sup>-3</sup> )	lin	ip
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)

# Pair Correlation Function - Preliminary

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



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