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:**

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

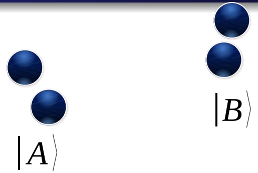
- **AFDMC:**

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

- Ψ_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, $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$, $\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, S_{ij} and $S_{ij} \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, where $S_{ij} = 3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$.

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

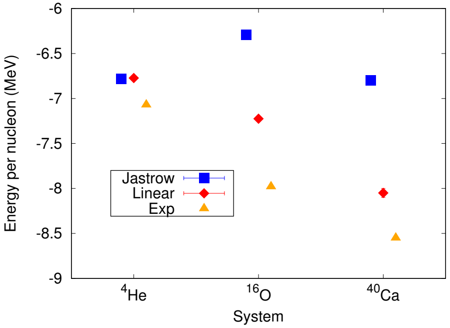
$$|\psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij})\right] \mathcal{S} \prod_{i<j} \left(1 + \sum_p f_p(r_{ij}) \mathcal{O}_{ij}^p\right) |\phi\rangle$$

- 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 $\mathcal{O}_{ij}$.

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



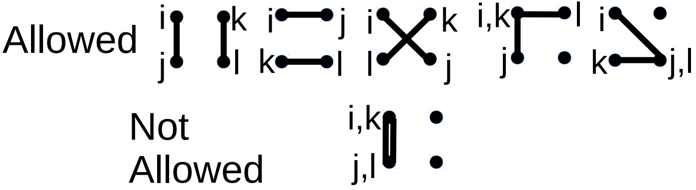
Jastrow: S. Gandolfi et al. *Phys. Rev. Lett.*, **99**, 022507, 2007.

Jastrow+Linear: S. Gandolfi et al. *Phys. Rev. C.*, **90**, 061306(R), 2014.

Quadratic Correlations

- Symmetrized product wave function up to quadratic order

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

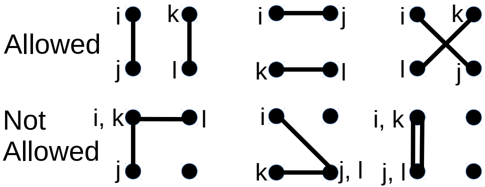


Independent Pair Quadratic Correlations

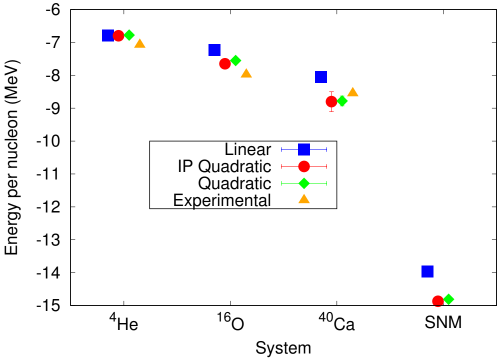
- Independent pair expansion to quadratic order

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

$$\left. + \sum_{i<j}\sum_{p} f_p(r_{ij})\mathcal{O}^p_{ij} \sum_{k<l,\mathrm{ip}}\sum_{q} f_q(r_{kl})\mathcal{O}^q_{kl}\right]|\phi\rangle$$



Results - AFDMC

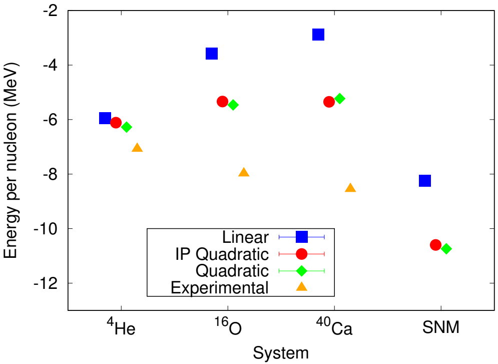


D. Lonardoni et al. *Phys. Rev. C.*, **97**, 044318, 2018.

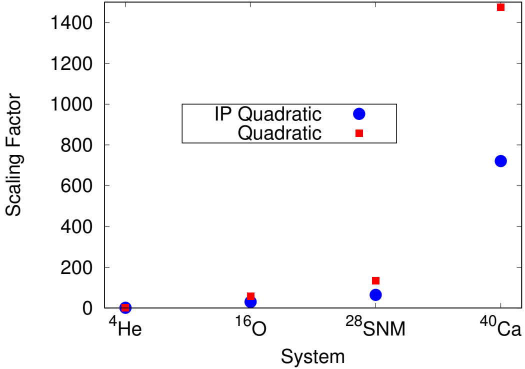
Table: Energy (*per nucleon) in MeV

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

Results - VMC


-2
-4
-6
-8
-10
-12
Energy per nucleon (MeV)
Linear
IP Quadratic
Quadratic
Experimental
^{4}He
^{16}O
^{40}Ca
SNM
System

Quadratic Correlation Cost



	^{4}He	^{16}O	SNM(28)	^{40}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

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ASU Arizona State University

XSEDE Extreme Science and Engineering Discovery Environment

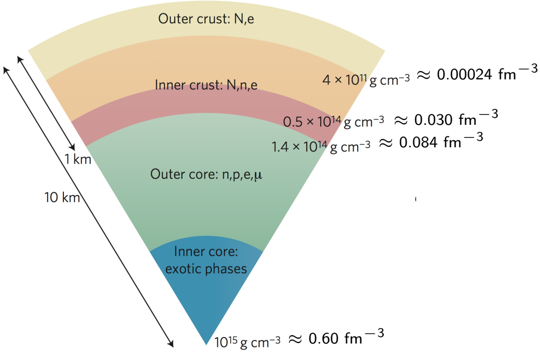
NSF

Extra Slides

Neutron Stars - Preliminary

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

$$E_\alpha = E_{\text{Nn+2p}} - E_{\text{(N-2)n}}$$



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

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

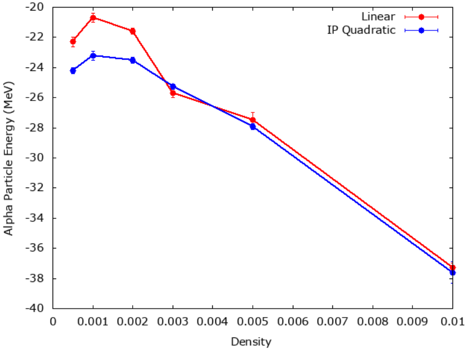
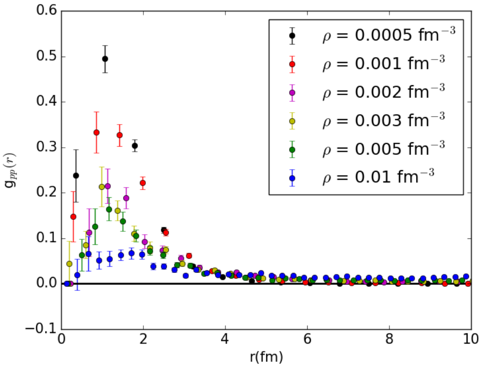


Table: Alpha energy in MeV

ρ (fm^{-3})	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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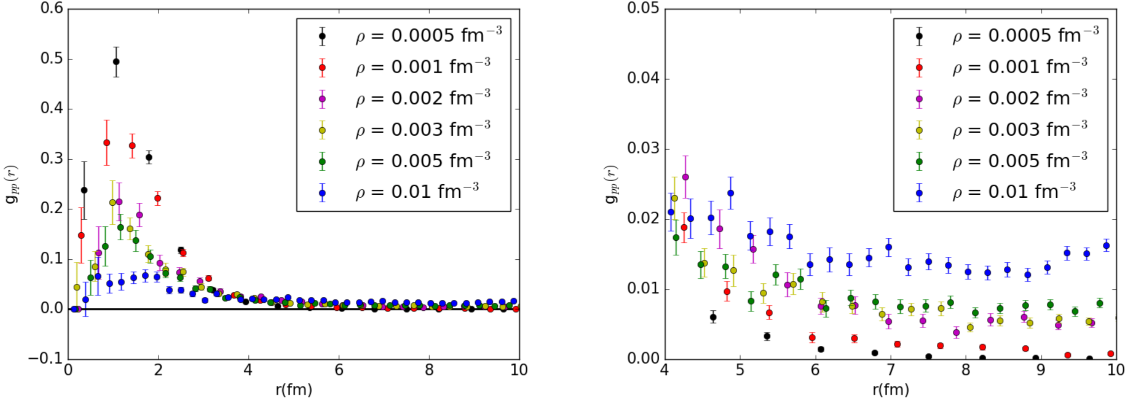

Variational Monte Carlo - Implementation

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 ξ 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 $\mathbf{R} \to \mathbf{R}'$, 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 $\mathrm{int}\,(w(\mathbf{R}') + \xi)$, where ξ is a uniform random number from $[0, 1]$.

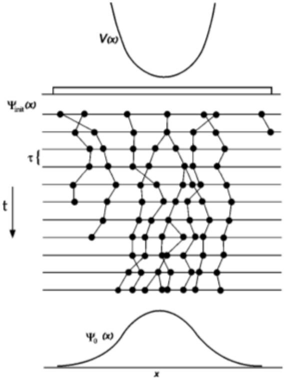

Figure: Reprinted from W.M.C. Foulkes et al. *Rev. Mod. Phys.*, 73:33-83, 2001.

Diffusion Monte Carlo - Short Time Propagator

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

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

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 χ 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 $w(\mathbf{R}') = \exp\left(-\left(E_L(\mathbf{R}') + E_L(\mathbf{R}) - 2E_0\right)\Delta\tau/2\right)$.
   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.