Alpha particle formation in neutron star crusts with an improved trial wave function for nuclear Quantum Monte Carlo

Cody L. Petrie
Advisor: Kevin Schmidt

Arizona State University
Tempe, AZ

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Outline

- Quantum Monte Carlo methods
- Improved trial wave function
- Alpha formation in nearly neutron matter - preliminary

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.

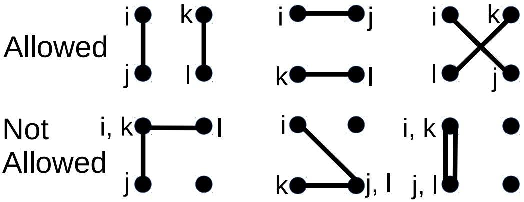
Slater Determinant

- 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.

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

Independent Pair Quadratic Correlations

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



Results

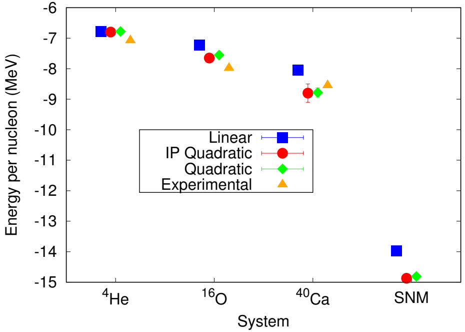


Table: Energy (*per nucleon) in MeV

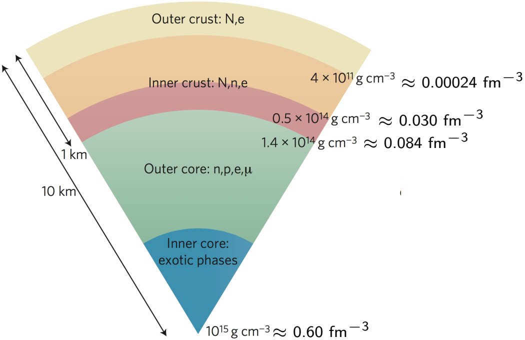
System	Linear	IP Quadratic	Quadratic	Experimental
^{4}He	-27.14(4)	-27.19(3)	-27.11(3)	-28.296
^{16}O	-115.7(9)	-122.4(1.5)	-120.8(1.3)	-127.62
^{40}Ca	-322(3)	-350(10)	-351(6)	-342.1
SNM*	-13.97(3)	-14.87(4)	-14.81(3)	

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

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

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

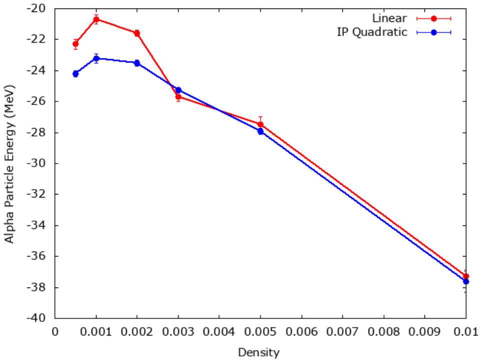
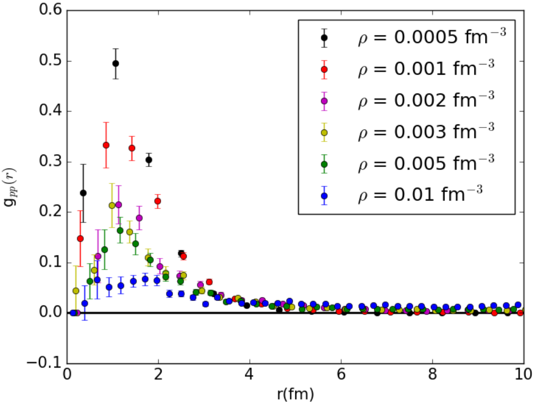


Table: Alpha energy in MeV

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

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



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.
- We have shown that our calculation can see what are probably alpha particles forming in mostly neutron matter around the density of neutron star crusts. These calculations appear to be even better when improved correlations are used.

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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 $[0, 1]$.

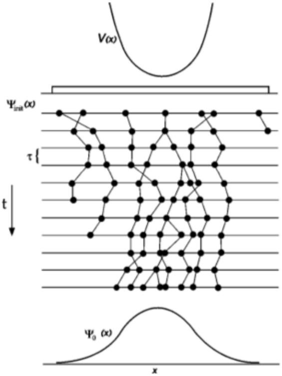


Figure: Reprinted from W.M.C. Foulkes et al. *Rev. Mod. Phys.*, 73:33-83, 2001.

Diffusion Monte Carlo - Short Time Propagator

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

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

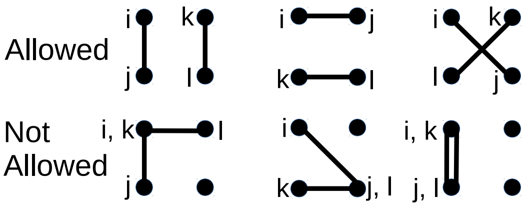
Diffusion Monte Carlo - Implementation

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.

Spin-Isospin Correlations

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

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



Spin Dependent Correlations

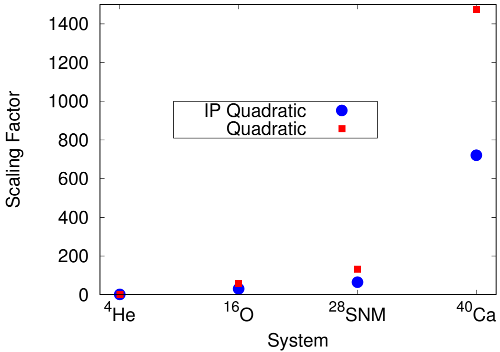
- Two spin dependent wave functions that are antisymmetric and obey cluster decomposition are the exponentially correlated and symmetrized product wave functions, where $\mathcal{O}_{ij}^p$ are the AV6 operators, $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$, $\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, 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.

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

Pair Correlation Function - Preliminary